

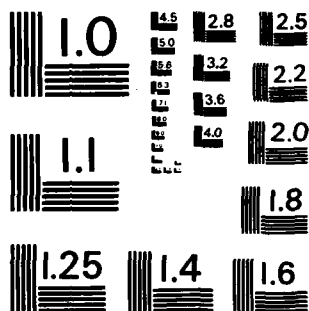
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AN IMPLICIT, WIGGLE-FREE, AND ACCURATE  
UPSTREAM FINITE-DIFFERENCE ALGORITHM  
FOR THE ONE-DIMENSIONAL  
TRANSPORT-DIFFUSION EQUATION

by

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20. ABSTRACT (Continued).

→ explicit scheme, the implicit method essentially doubles the useful, stable range of application with comparable accuracy.

Because of these significant improvements for one-dimensional problems, it is strongly recommended that the implicit method be extended to two dimensions.

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## PREFACE

This report was prepared by Dr. David R. Basco, Department of Civil Engineering, Texas A&M University Research Foundation, for the U. S. Army Engineer Waterways Experiment Station (WES) under Contract No. DACW39-81-M-4377 dated 19 August 1981. The study was sponsored by the Office, Chief of Engineers, under the Environmental Impact Research Program (EIRP) Work Unit 31730. The purpose of the report was to investigate the formulation and stability of implicit formulations of QUICKEST. The report is directed toward personnel with an understanding of finite differences.

The study was monitored at WES by Mr. Ross Hall, Environmental Research and Simulation Division (ERSD), Environmental Laboratory (EL). Mr. Donald Robey, Chief, ERSD, and Dr. John Harrison, Chief, EL, provided supervision. Dr. Roger Saucier was Program Manager, EIRP; Mr. John Bushman was Technical Monitor.

Commander and Director of WES during report preparation was COL Tilford C. Creel, CE. Technical Director was Mr. F. R. Brown.

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## TABLE OF CONTENTS

	<u>Page</u>
PREFACE . . . . .	1
LIST OF FIGURES . . . . .	3
NOMENCLATURE . . . . .	5
PART I: INTRODUCTION . . . . .	7
PART II: EXPLICIT LEONARD ALGORITHM (QUICKEST) . . . . .	9
Explicit Operator . . . . .	10
Equivalence to a Higher Order Accuracy Method . . . . .	11
Linear Stability Analysis . . . . .	15
Verification . . . . .	19
Wiggles . . . . .	23
PART III: IMPLICIT ALGORITHMS . . . . .	27
Implicit Leonard Algorithm for Transport-Diffusion (QUICKIST) . . . . .	27
Fully Centered, Implicit Algorithm (QUICKOST) . . . . .	37
PART IV: CONCLUSIONS AND RECOMMENDATIONS . . . . .	47
Conclusions . . . . .	47
Recommendations . . . . .	47
REFERENCES . . . . .	49
APPENDIX A: DERIVATION OF QUICKOST 2 . . . . .	A1

# LIST OF FIGURES

<u>Figure</u>		<u>Page</u>
1	Schematic of QUICKEST algorithm for flow from left to right . . . . .	9
2	Amplitude portraits of QUICKEST for $C = 1.0, 0.9,$ and $0.5$ for pure advection ( $\Gamma = 0$ ) . . . . .	17
3	Stability range of QUICKEST method in $(\Gamma, C)$ plane as mapped by Leonard (1979) . . . . .	17
4	Amplitude and phase portraits of QUICKEST and QUICKIST (implicit) schemes when $C = 0.5$ , $\Gamma = 1.1$ . . . . .	20
5	Amplitude and phase portraits of QUICKEST and QUICKIST (implicit) schemes when $C = 0.5$ , $\Gamma = 1.2$ . . . . .	21
6	Contour lines of equal RMS difference values (iso-amplitudes) on the $(\Gamma, C)$ plane for QUICKEST . . . . .	22
7	Propagation test results for pure advection case using periodic boundary conditions and QUICKEST algorithm with $C = 0.5$ . . . . .	23
8	Example of wiggle instability for implicit, centered advection of test triangle with periodic boundary conditions . . . . .	25
9	Suppression of wiggle instability when $P_{\Delta} < 2$ for implicit, centered advection of test triangle . . . . .	26
10	Amplitude portrait for QUICKEST versus QUICKIST schemes when $C = 0.5$ , $\Gamma = 0$ . . . . .	31
11	Amplitude and phase portraits for QUICKEST and QUICKIST schemes when $C = 1.0$ , $\Gamma = 0$ . . . . .	32
12	Amplitude response for pure diffusion ( $c = 0$ ) when $\Gamma = 1/6$ for both QUICKEST and QUICKIST schemes . . . . .	33
13	Stable range of QUICKIST method in $(\Gamma, C)$ plane as determined in this study . . . . .	34
14	Iso-amplitude lines of equal RMS difference values in $(\Gamma, C)$ plane for QUICKIST . . . . .	35
15	Propagation tests for pure advection using periodic boundary conditions and QUICKIST algorithm . . . . .	36
16	Schematic of operator for QUICKEST scheme determination . . . . .	38
17	Amplitude and phase portraits for QUICKEST scheme and pure advection ( $\Gamma = 0$ ) case when $C = 0.5$ and $1.0$ . . . . .	42



# LIST OF FIGURES (Continued)

<u>Figure</u>		<u>Page</u>
18	Iso-amplitude plot for QUICK0ST with stable range also shown . . . . .	43
19	Propagation test results for pure advection case using periodic boundary conditions and QUICK0ST algorithm . . .	44
20	Propagation test results for example with some physical diffusion present ( $\Gamma = 0.1$ ) comparing explicit (dots) and implicit (triangles) QUICK0ST algorithms . . . . .	45
21	Propagation test results for narrow triangle ( $JW = 2$ ) and physical diffusion ( $\Gamma = 0.1$ ) comparing QUICKEST (dots) and QUICK0ST (triangles) algorithm when $C = 0.5$ , $\Gamma = 0.1$ , $P_{\Delta} = 5$ after 200 time steps . . . . .	46

# NOMENCLATURE

a,b,k,h	Variables in two-dimensional Taylor series expansion method
A	Amplification factor in linear stability method, A = modulus; coefficient in QUICK method of Leonard (1979)
A,B,C1,D,E,F,H	Coefficients in implicit, finite-difference methods
C	Courant number
CURV	Curvature
e	A subscript meaning <u>exact</u> equation
GRAD	Gradient
H.O.T.	Higher order truncation error terms
i	Space step index
o	
Π	Imaginary number index
JW	One half the base width of the test triangle
κ	Wave number, $2\pi/L$
K	Diffusion (dispersion) coefficient
ℓ	Left side wall value as subscript
L	Wave length
n	Time step index as superscript; also number of Taylor series terms
N	Total number of grid points in one full wave length
NN	Total number of time steps
P <sub>Δ</sub>	Péclet number
Q	Phase ratio
r	Right side wall value as subscript
R <sub>e</sub>	Exact continuum response function
RMS	Root-mean-square value
t	Time; as subscript means time differentiation
Δt	Time step
u	Velocity
x	Space coordinate; as subscript means space differentiation
Δx	Space step
①, ②, ③, etc.	Truncation error terms

1-D	One-dimensional
2-D	Two-dimensional
$\alpha$	Dimensionless wave number
$\Gamma$	Dimensionless diffusion coefficient (the diffusion number)
$\theta$	Weighting factor, $0 \leq \theta \leq 1$ in implicit schemes
$\phi$	Dependent variables

AN IMPLICIT, WIGGLE-FREE, AND ACCURATE UPSTREAM  
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PART I: INTRODUCTION

1. Implicit finite-difference algorithms use more than one unknown variable at the next time level ( $n+1$ ) in the calculation. They thereby require the simultaneous solution of many equations at time ( $n+1$ ) in order to advance the computation for marching-type, initial value/boundary value problems.

2. In general, implicit schemes have better stability properties than explicit schemes. For propagation-dominated problems, this means running with Courant numbers greater than unity to use more economic time steps in the computation. In general, the price paid is less accuracy and larger Central Processing Unit (CPU) times on the computer. In addition, implicit schemes require a prescribed order or direction of the computation in the space of the independent variables. This can be called the algorithmic structure of the scheme (Abbott 1979). Use of an inappropriate structure will result in an ill-posed problem and unstable solution.

3. Engineers require robust schemes in their computational systems to provide greater flexibility in use, yet maintain acceptable standards of accuracy over a wide variety of conditions. Properly designed implicit schemes have met these needs in many aspects of Computational Hydraulics.

4. For transport-diffusion computations, Leonard (1979) has developed the explicit QUICKEST modeling procedure. It avoids the "wobble" instability problem associated with central differencing of the advection term. It also eliminates the inaccuracies of numerical diffusion resulting when only first-order, upstream differencing procedures are employed. The purpose of this research effort was to develop and study numerical properties of an implicit algorithm consistent with the Leonard (1979) scheme for the one-dimensional transport-diffusion equation.

5. Part II of this report reviews the explicit scheme of Leonard (1979) and proves its equivalence to first-order differences with judicious removal of the truncation error terms. In Part III, two implicit schemes are developed and their characteristics are investigated using linear stability analysis methods and standard numerical tests. Both implicit methods are then compared with the explicit Leonard scheme. Conclusions and recommendations follow in Part IV.

## PART II: EXPLICIT LEONARD ALGORITHM (QUICKEST)

6. It is highly instructive to briefly review Leonard's (1979) explicit scheme for unsteady transport diffusion, which is labeled QUICKEST (quadratic upstream interpolation for convective kinematics with estimated streaming terms). Consider the differential equation

$$\phi_t + u\phi_x = K\phi_{xx} \quad u, K \text{ real constants} \quad (1)$$

together with appropriate initial and boundary conditions.\* A scalar quantity  $\phi$  is convected by constant velocity  $u$  and diffused by a constant diffusion coefficient  $K$  in one space dimension. A source term could also be added, if necessary.

7. For the finite-difference grid shown in Figure 1, Leonard (1979) proposed using a basic, three-point, upstream-weighted, quadratic interpolation scheme for "wall" values  $\phi_r$  (right) and  $\phi_l$  (left) of a control volume when  $u$  is positive to the right. For steady-state conditions, Leonard took

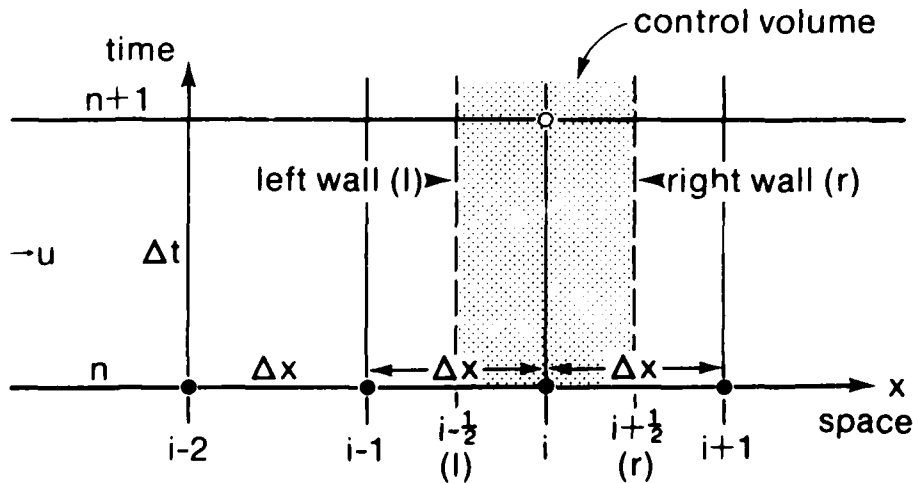


Figure 1. Schematic of QUICKEST algorithm for flow from left to right

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\* See "Nomenclature" on page 5 for definitions of symbols and abbreviations.

$$\phi_r = \phi_{i+1/2} = 1/2(\phi_{i+1} + \phi_i) - A(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \quad (2)$$

$$\phi_\ell = \phi_{i-1/2} = 1/2(\phi_i + \phi_{i-1}) - A(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \quad (3)$$

with  $A = 1/8$  for steady flows (QUICK algorithm).

8. For unsteady-state conditions, Equations 2 and 3 were incorporated in an exact integral formulation where average wall values over time increment  $\Delta t$  were employed. Complete details are beyond the intended scope of this review.

#### Explicit Operator (QUICKEST)

9. The resultant explicit, finite-difference operator for the QUICKEST algorithm becomes (Leonard 1979, p. 80, Equation 57)

$$\begin{aligned} \phi_i^{n+1} = \phi_i^n - C \left\{ \begin{aligned} &\left[ 1/2(\phi_{i+1}^n + \phi_i^n) - \frac{\Delta x}{2} C \cdot \text{GRAD}_r - \frac{\Delta x^2}{6} (1 - C^2 - 3\Gamma) \text{CURV}_r \right] \\ &- \left[ 1/2(\phi_i^n + \phi_{i-1}^n) - \frac{\Delta x}{2} C \cdot \text{GRAD}_\ell - \frac{\Delta x^2}{6} (1 - C^2 - 3\Gamma) \text{CURV}_\ell \right] \end{aligned} \right\} \quad (4) \\ + \Gamma \left[ \left( \Delta x \text{GRAD}_r - \frac{\Delta x^2}{2} C \cdot \text{CURV}_r \right) - \left( \Delta x \text{GRAD}_\ell - \frac{\Delta x^2}{2} C \cdot \text{CURV}_\ell \right) \right] \end{aligned}$$

where:

$$C = \frac{u\Delta t}{\Delta x} = \text{the Courant Number}$$

$$\Gamma = \frac{K\Delta t}{\Delta x^2} = \text{the dimensionless diffusion coefficient, or the diffusion number}$$

$$\text{GRAD}_r = \frac{\phi_{i+1}^n - \phi_i^n}{\Delta x}$$

$$\text{CURV}_r = \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}$$

$$\text{GRAD}_{\ell} = \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$$

$$\text{CURV}_{\ell} = \frac{\phi_i^n - 2\phi_{i-1}^n + \phi_{i-2}^n}{\Delta x^2}$$

for flow from left to right for both walls ( $r$  = right;  $\ell$  = left). Note that for this case, both curvature terms  $\text{CURV}$  are actually centered upstream by one-half increment and not at  $r$  or  $\ell$  as indicated. This is a key aspect of the QUICKEST scheme. In Equation 4, the physical diffusion is calculated using a standard, centered, second difference operator at point  $i$ . The overall (global) truncation error is third order in space, and the scheme gives a conservative formulation with no wiggle instabilities present.

#### Equivalence to a Higher Order Accuracy Method

10. As shall be demonstrated below, QUICKEST is equivalent to a forward-time, centered-space (FTCS) scheme in which the truncation errors resulting from all terms are subtracted out in a prescribed manner.

11. From a Taylor's series expansion about point  $(i,n)$  in Figure 1, one obtains the finite-difference analog to Equation 1.

$$\begin{aligned} & \textcircled{1} \left[ \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} \right] + u \textcircled{3} \left[ \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} \right] = K \textcircled{5} \left[ \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \right] \\ & + \textcircled{2} \left[ \frac{\Delta t}{2!} \phi_{tt} + \frac{\Delta t^2}{3!} \phi_{ttt} + \frac{\Delta t^3}{4!} \phi_{tttt} + \text{H.O.T.} \right]_i^n \\ & + u \textcircled{4} \left[ \frac{\Delta x^2}{3!} \phi_{xxx} + \frac{\Delta x^4}{5!} \phi_{xxxxx} + \text{H.O.T.} \right]_i^n \end{aligned}$$



$$\textcircled{6} \quad - K \left[ \frac{2\Delta x^2}{4!} \phi_{xxxx} + \frac{2\Delta x^4}{6!} \phi_{xxxxxx} + \text{H.O.T.} \right]_1^n \quad (5)$$

A forward-time difference (term  $\textcircled{1}$ ) and a centered-space difference (term  $\textcircled{3}$ ) are employed along with a centered, second difference (term  $\textcircled{5}$ ) for the diffusion. The bracketed terms  $\textcircled{2}$ ,  $\textcircled{4}$ , and  $\textcircled{6}$  are the truncation errors associated with terms  $\textcircled{1}$ ,  $\textcircled{3}$ , and  $\textcircled{5}$ , respectively.

12. To eliminate the time derivatives in  $\textcircled{2}$ , Equation 1 can be further differentiated in time and space to yield

$$\phi_{tt} = u^2 \phi_{xx} - 2uK\phi_{xxx} \quad (6)$$

$$\phi_{ttt} = -u^3 \phi_{xxx} \quad (7)$$

and

$$\phi_{tx} = -u\phi_{xx} + K\phi_{xxx} \quad (a) \quad (8)$$

$$\phi_{xtt} = u^2 \phi_{xxx} \quad (b)$$

when 4th derivatives are neglected. Equation 8 will be used later in this report. Substituting Equations 6 and 7 into 5 and grouping like-ordered differentials gives

$$\begin{aligned} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u \left[ \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} \right] &= K \left[ \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \right] \\ &+ \frac{u^2 \Delta t}{2!} [\phi_{xx}]_1^n + \left( \frac{u\Delta x^2}{6} - \frac{u^3 \Delta t^2}{6} - \frac{2uK\Delta t}{2} \right) [\phi_{xxx}]_1^n \\ &+ \left[ \frac{\Delta t^3}{4} \phi_{tttt} - \frac{2K\Delta x^2}{4!} \phi_{xxxx} + \text{H.O.T.} \right]_1^n \end{aligned} \quad (9)$$

The last bracketed term in Equation 9 is the truncation error

$O(\Delta t^3, \Delta x^2)$  and contains fourth-order and higher differentials which are neglected. Multiplying through by  $\Delta t$  and clearing all n-level terms to the right-hand side (RHS) gives

$$\begin{aligned} \phi_i^{n+1} = & \phi_i^n - \frac{C}{2} (\phi_{i+1}^n - \phi_{i-1}^n) + \Gamma (\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n) \\ & + C \left[ \frac{C\Delta x^2}{2} \phi_{xx} + \frac{\Delta x^2}{6} (\Delta x - C^2\Delta x - 6\Gamma\Delta x) \phi_{xxx} \right]_i^n \end{aligned} \quad (10)$$

The bracketed term in Equation 10 is the remaining truncation error below  $\phi_{xxx}$  and the method in which it is finite-differenced is central to the equivalency of Equations 4 and 10.

13. Using the terms defined by Leonard (1979) in Equation 4 gives

$$\begin{aligned} (\phi_{xx})_i^n &= \frac{\text{GRAD}_r - \text{GRAD}_\ell}{\Delta x} = \frac{\left[ \frac{\phi_{i+1}^n - \phi_i^n}{\Delta x} \right] - \left[ \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} \right]}{\Delta x} \\ &= \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \end{aligned}$$

or

$$\Delta x (\phi_{xx})_i^n = \text{GRAD}_r - \text{GRAD}_\ell \quad (11)$$

Thus, for  $\phi_{xx}$ , the centering is precisely at  $(i, n)$  as required by Equation 10. Now, if the centering of  $\phi_{xxx}$  is judiciously moved upstream to  $(i - 1/2, n)$ , it is assumed that

$$\begin{aligned} (\phi_{xxx})_i^n &\approx (\phi_{xxx})_{i-1/2}^n = \frac{\text{CURV}_r - \text{CURV}_\ell}{\Delta x} \\ &= \frac{\left[ \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \right]_i^n - \left[ \frac{\phi_i^n - 2\phi_{i-1}^n + \phi_{i-2}^n}{\Delta x^2} \right]_{i-1}^n}{\Delta x} \end{aligned}$$

$$= \frac{\phi_{i+1}^n - 3\phi_i^n + 3\phi_{i-1}^n - \phi_{i-2}^n}{\Delta x^3}$$

or

$$\Delta x \left( \phi_{xxx} \right)_i^n \approx \Delta x \left( \phi_{xxx} \right)_{i-1/2}^n = \text{CURV}_r - \text{CURV}_\ell \quad (12)$$

The identity

$$\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2} \equiv 1/2 \left[ \phi_i^n + \phi_{i+1}^n \right] - 1/2 \left[ \phi_i^n + \phi_{i-1}^n \right] \quad (13)$$

is also required.

14. Putting Equations 11, 12, and 13 into Equation 10 gives

$$\begin{aligned} \phi_i^{n+1} = & \phi_i^n - c \left[ 1/2 \left( \phi_i^n + \phi_{i+1}^n \right) - 1/2 \left( \phi_i^n + \phi_{i-1}^n \right) \right] + \Gamma \left[ \left( \Delta x \text{GRAD}_r \right) \right. \\ & \left. - \left( \Delta x \text{GRAD}_\ell \right) \right] + c \left[ \frac{c}{2} \Delta x \left( \text{GRAD}_r - \text{GRAD}_\ell \right) \right. \\ & \left. + \frac{\Delta x^2}{6} \left( 1 - c^2 - 6\Gamma \right) \left( \text{CURV}_r - \text{CURV}_\ell \right) \right] \quad (14) \end{aligned}$$

The final trick to recover the form given by Leonard is to split the last term in Equation 14 simply by taking

$$-6\Gamma = -3\Gamma - 3\Gamma$$

and through some further rearrangement. Equation 4 is thus recovered and the derivation is complete.

15. For programming purposes, a much simpler version can be obtained by inserting the difference Equations 11 and 12 for  $\phi_{xx}$  and  $\phi_{xxx}$ , respectively. After grouping all like terms, one obtains

$$\begin{aligned}
\phi_i^{n+1} = & \phi_i^n + \left[ -\frac{C}{2} + \Gamma + \frac{C^2}{2} + \frac{C}{6} (1 - C^2 - 6\Gamma) \right] \phi_{i+1}^n \\
& - \left[ 2\Gamma + C^2 + \frac{C}{2} (1 - C^2 - 6\Gamma) \right] \phi_i^n + \left[ \frac{C}{2} + \Gamma + \frac{C^2}{2} \right. \\
& \left. + \frac{C}{2} (1 - C^2 - 6\Gamma) \right] \phi_{i-1}^n - \left[ \frac{C}{6} (1 - C^2 - 6\Gamma) \right] \phi_{i-2}^n \quad (15)
\end{aligned}$$

16. The algorithm for QUICKEST does reduce to that given by Leonard (1979) for the steady-state algorithm (QUICK) when term (2) for time derivative truncation error is omitted. Thus QUICKEST implicitly takes  $A = 1/6$  in Equations 2 and 3. Other reduced forms are

Pure Advection ( $\Gamma = 0$ )

$$\begin{aligned}
\phi_i^{n+1} = & \phi_i^n - \frac{C}{6} (C^2 - 3C + 2) \phi_{i+1}^n + \frac{C}{2} (C^2 - 2C - 1) \phi_i^n \\
& - \frac{C}{2} (C^2 - C - 2) \phi_{i-1}^n + \frac{C}{6} (C^2 - 1) \phi_{i-2}^n \quad (16)
\end{aligned}$$

Pure Diffusion ( $C = 0$ )

$$\phi_i^{n+1} = \phi_i^n + \Gamma (\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n) \quad (17)$$

When  $\Gamma = 0$  and  $C = +1$ , Equation 16 reduces to  $\phi_i^{n+1} = \phi_{i-1}^n$  or point-to-point transport for an exact result.

### Linear Stability Analysis

17. As a further review and check of these results, a von Neumann linear stability analysis was made of Equation 15. This resulted in the following expression for the amplification factor  $A$

$$\begin{aligned}
A(\alpha) = & 1 + 2(\Gamma + \frac{1}{2} C^2)(\cos \alpha - 1) \\
& + \left[ \frac{1}{6} C(1 - C^2 - 6\Gamma)(4 \cos \alpha - 3 - \cos 2\alpha) \right] \\
& - \frac{1}{6} C \left[ \sin \alpha + \frac{1}{6} (1 - C^2 - 6\Gamma)(2 \sin \alpha - \sin 2\alpha) \right] \quad (18)
\end{aligned}$$

where:

$\alpha = \kappa \Delta x =$  the dimensionless wave number

$\kappa =$  the wave number  $\frac{2\pi}{L}$

$\alpha = \frac{2\pi}{N}$

$N =$  the number of grid intervals per wave length  $L$

$\Pi =$  the imaginary number index

Equation 18 is identical to that derived by Leonard (1979, p. 81, Equation 59), which gives further confidence in these results.

18. An example amplitude portrait for the pure advection case is shown in Figure 2 for three values of the Courant number. The modulus of  $A$  versus  $\alpha$  plot (Figure 2a) gives more resolution for the higher wave numbers ( $\alpha \rightarrow \pi$ ) and consequently has been employed for all subsequent portraits. No phase errors exist for  $C = 0.5$  and  $1.0$  ( $\Gamma = 0$ ).

19. The complete stability range in the  $(\Gamma, C)$  plane for the QUICKEST algorithm as mapped by Leonard (1979) is reproduced in Figure 3. Lines of constant Péclet number  $P_\Delta$  defined as

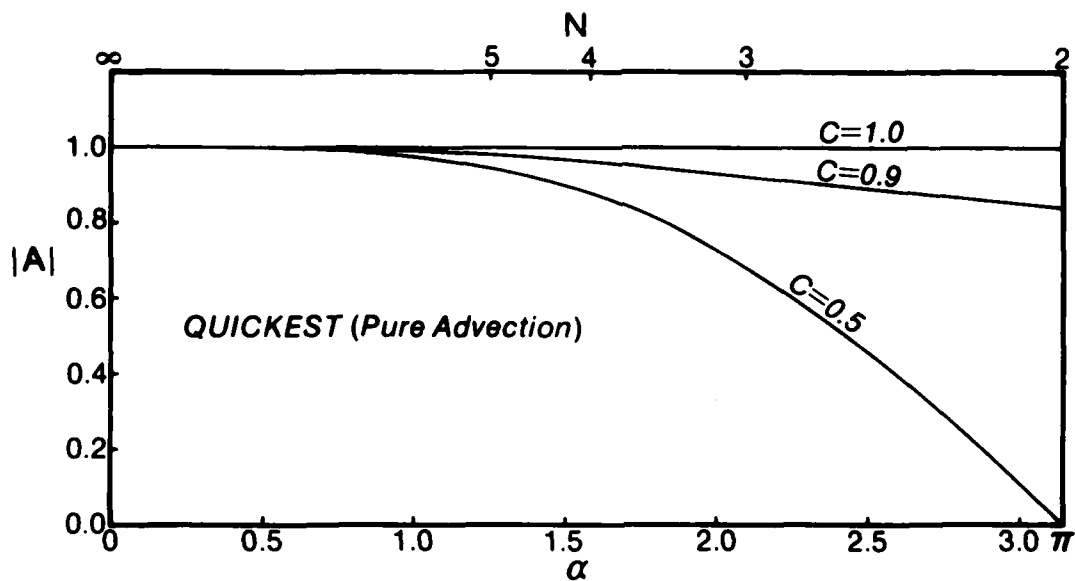
$$P_\Delta = \frac{C}{\Gamma} \quad (19)$$

are also shown. When  $\Gamma = 0$  ( $P_\Delta = \infty$ ), the QUICKEST scheme is unstable when  $1 < C < 2$  and also for  $C > 2$ . The scheme is stable for all other  $\Gamma, C$  values within the space shown with the  $P_\Delta$  lines. Although this explicit scheme is stable for a considerable range above  $C = 1$ , it also is unstable in a "corner" beyond  $\Gamma = 0.5$  and below  $C = 0.5$ . It would be anticipated that an implicit version would eliminate this unstable corner.

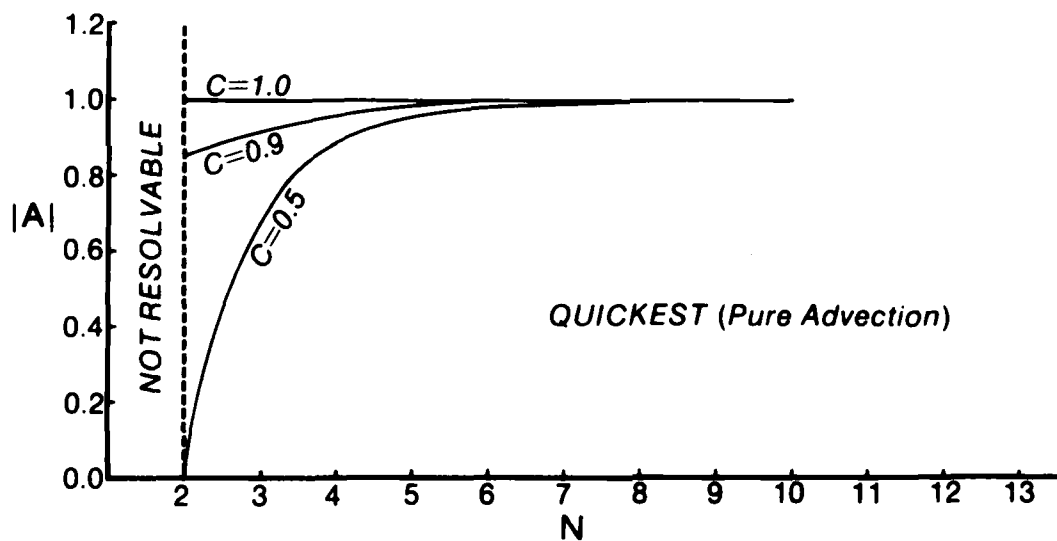
20. But Figure 3 reveals nothing about the accuracy of the scheme. For the continuum Equation 1, the exact amplitude response function  $R_e(\alpha)$  is given by

$$R_e(\alpha) = \exp(-\Gamma \alpha^2) \quad (20)$$

since the modulus for pure advection alone is unity over all  $\alpha$ . The exact phase ratio  $Q_e$  is also unity for all  $\alpha$  since pure diffusion has



(a) When wave number space is defined by  $\alpha$ .



(b) When wave number space is defined by  $N$ .

Figure 2. Amplitude portraits of QUICKEST for  $C = 1.0$ , 0.9, and 0.5 for pure advection ( $\Gamma = 0$ )

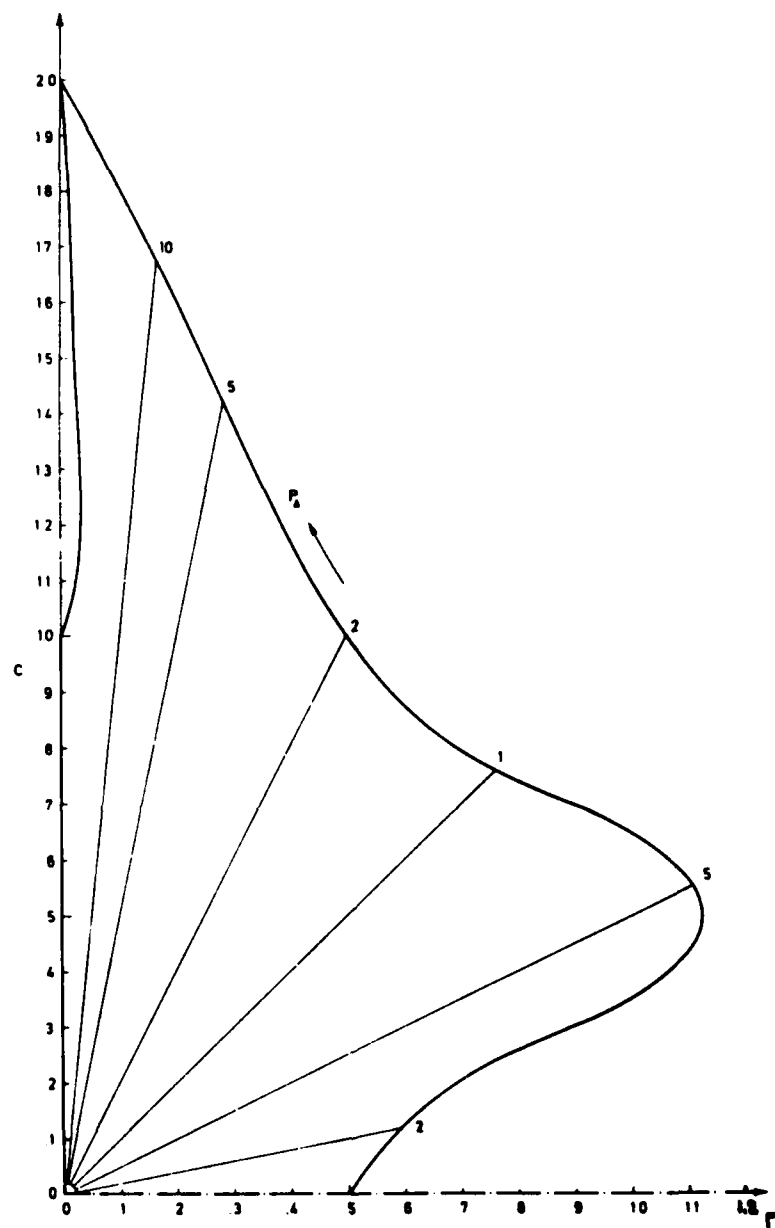


Figure 3. Stability range of QUICKEST method in  $(\Gamma, C)$  plane as mapped by Leonard (1979). Note that the scheme is unstable for  $1 < C < 2$  and again for  $C > 2$  when  $\Gamma = 0$

no phase properties. Examples of the accuracy characteristics of QUICK-EST are presented in Figure 4 when  $C = 0.5$ ,  $\Gamma = 1.1$  and in Figure 5 for  $C = 0.5$ ,  $\Gamma = 1.2$ . The exact response in both cases is also presented. For the stable case (1.1, 0.5), large differences occur for both  $|A|$  and  $Q$  at higher wave numbers meaning low accuracy for these short wave components. The unstable case (1.2, 0.5) is clearly revealed by the amplitude portrait in Figure 5.

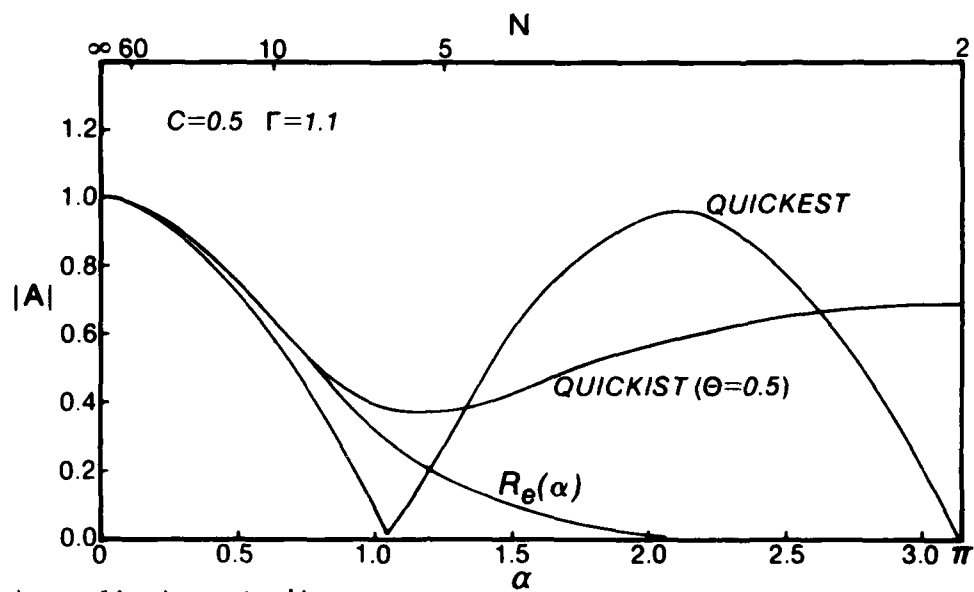
21. It would be very beneficial to characterize the accuracy of QUICKEST by one number over the entire  $(\Gamma, C)$  plane. To do this, the root-mean-square (RMS) value of the differences between continuum (exact) and discrete (approximate) responses was computed using 59 values equally spaced in  $N$ . Iso-RMS "difference" lines were then constructed to give the "contour" type plot for amplitude response presented in Figure 6. The weighted-average RMS difference value for the stable area (also traced on Figure 6) is 0.0568. In  $N$ -space, this RMS norm was found dependent on the number of differences employed. Further research is needed to refine this approach.

### Verification

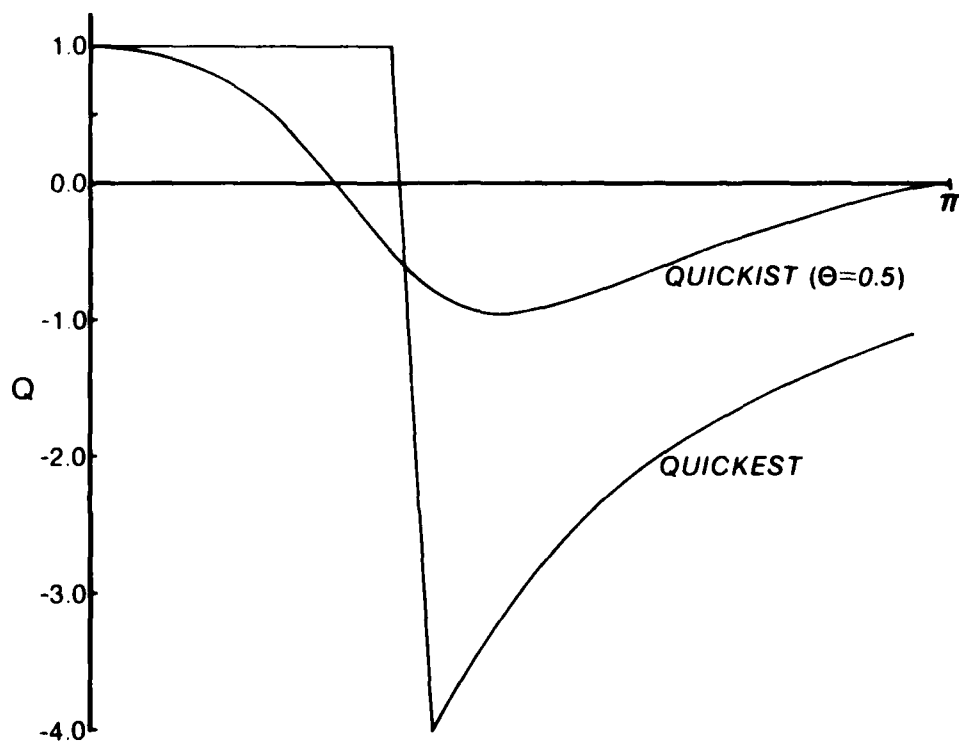
22. A convenient and informative numerical test for verification of transport-diffusion schemes is the propagation of test triangles with periodic boundary conditions. Since numerical diffusion and convective phase errors are of primary concern, these tests are made with no physical diffusion ( $\Gamma = 0$ ) present. Two examples are shown in Figure 7. Triangles with peak of 1.0 unit centered at  $i = 50$  on a 100-unit grid and half-base widths of 20 units (Figure 7a) and 2 units (Figure 7b) are propagated with  $C = +0.5$  (left to right). With this Courant number and using periodic boundary conditions, 200 time steps are needed to return the triangle to its initial position shown.

23. The points shown in Figures 7a and 7b are results using the QUICKEST algorithm after 200 time steps. No phase errors are indicated, which confirms the von Neumann analysis. However, numerical amplitude errors for high wave number components cause the peak to be damped,



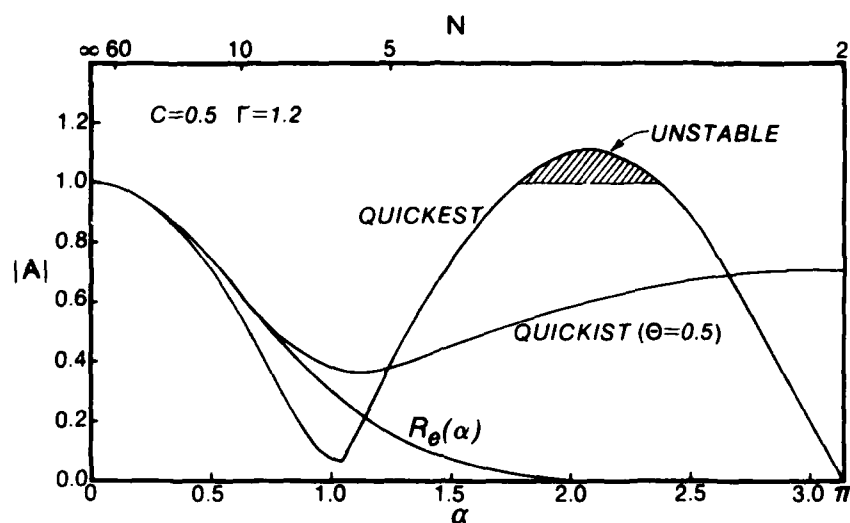


(a) Amplitude portrait.

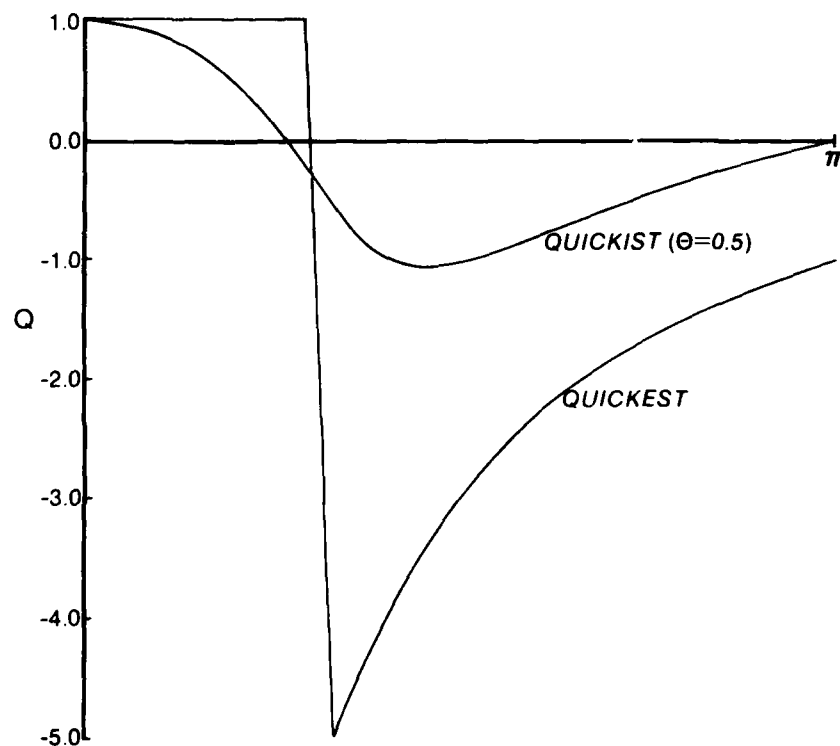


(b) Phase portrait.

Figure 4. Amplitude and phase portraits of QUICKEST and QUICKIST (implicit) schemes when  $C = 0.5$ ,  $\Gamma = 1.1$



(a) Amplitude portrait.



(b) Phase portrait.

Figure 5. Amplitude and phase portraits of QUICKEST and QUICKIST (implicit) schemes when  $C = 0.5$ ,  $\Gamma = 1.2$ .  
Explicit QUICKEST is unstable

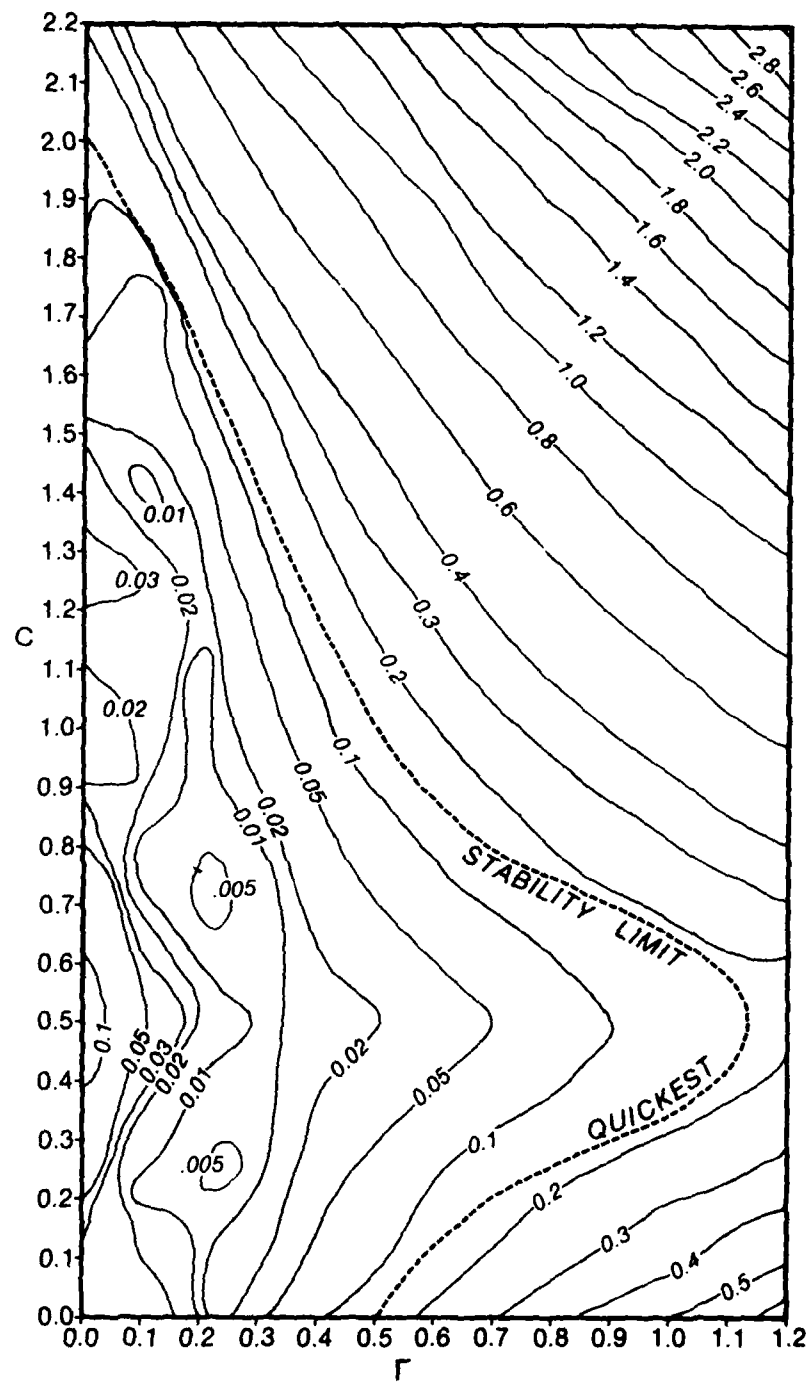
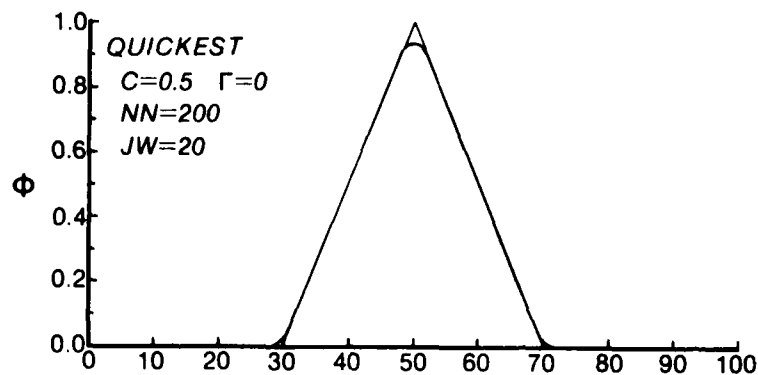
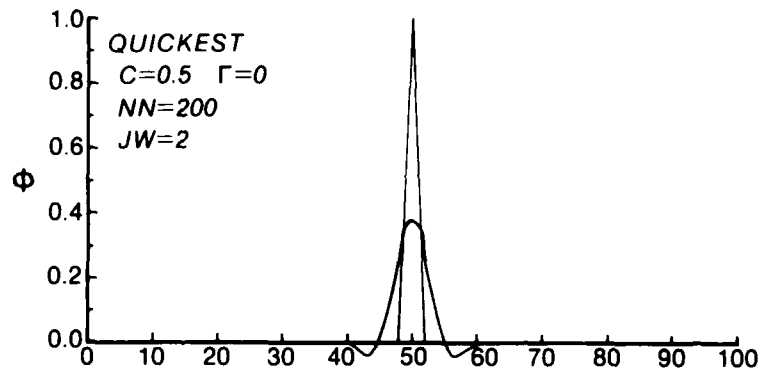


Figure 6. Contour lines of equal RMS difference values (iso-amplitudes) on the ( $\Gamma$ ,  $C$ ) plane for QUICKEST. Stability range also shown



(a) Wide triangle with half-base width of 20 units.



(b) Narrow triangle with half-base width of 2 units.

Figure 7. Propagation test results for pure advection case using periodic boundary conditions and QUICKEST algorithm with  $C = 0.5$

especially for the "spiked" triangle ( $JW = 2$ ) example. The damping of the wider triangle ( $JW = 20$ ) is relatively minor when compared with that produced by many first-order finite-difference schemes (see, e.g., Reid and Basco (1981) for other examples).

#### Wiggles

24. Wiggles as defined by Leonard (1979) are

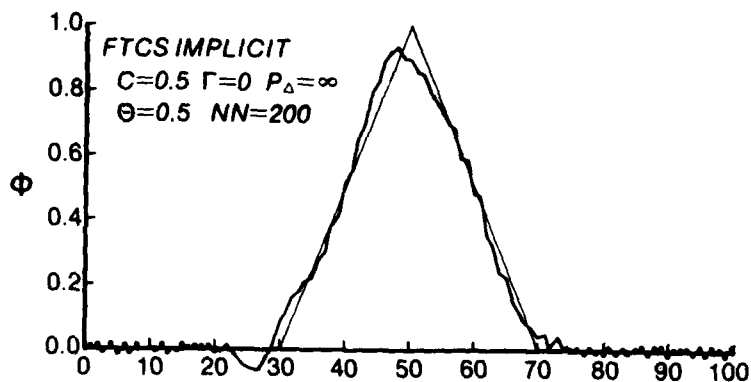
"...spatially decaying or growing oscillations of wavelength  $2\Delta x$  (i.e.  $\alpha = \pi$ ,  $N = 2$ ) - typical of central difference solutions of the...convective-diffusion problem for  $P_\Delta > 2$  .

...Interestingly enough, the criterion for the absence of wiggles,  $P_{\Delta} \leq 2$ , is not a stability condition in the von Neumann sense...." (p. 63)

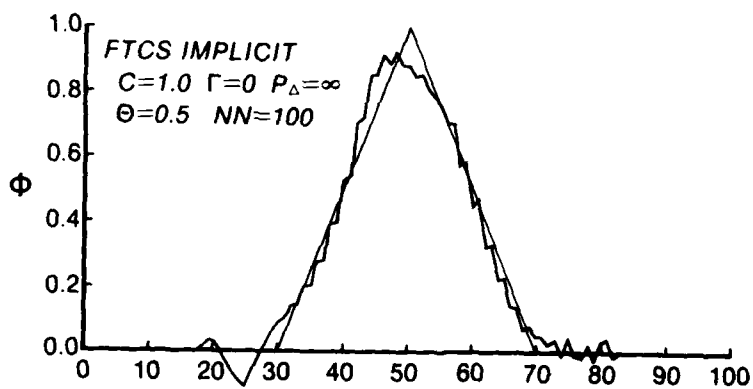
Roache (1977) discusses this as the "zero-overshoot" requirement while Abbott (1979) mentions "zig-zagging" of free-surface flow schemes. A full discussion of the sensitivity of the advection term for various schemes and sensitivity requirements to prevent wiggles is found in Leonard (1979). Upstream differencing of the advection term always prevents wiggles.

25. To further examine the wiggle problem for centered convection schemes, an implicit FTCS scheme was developed with no attempt to remove the truncation errors. An implicit scheme is necessary for stability since the explicit FTCS scheme for pure advection is always unstable. The advection term is centered in space and weighted between  $n$  and  $n + 1$  time levels by a weighting factor  $\theta$  ( $0 < \theta \leq 1$ ). The usual case employed  $\theta = 1/2$  to give the  $\sigma(\Delta t^2, \Delta x^2)$  for the truncation error.

26. A linear stability analysis proved the scheme stable for all  $(\Gamma, C)$  values when  $\theta \geq 0.5$ . Some phase errors existed, but  $|A| \equiv 1$  for all  $\alpha$  when  $C = 0.5$  and  $1.0$  ( $\theta = 1/2$ ). Propagation test results for the wide shape are shown in Figure 8. Clearly, an oscillation of length  $2\Delta x$  is present and can only be explained as a "wiggle" instability of central differencing since  $P_{\Delta} = \infty$  ( $\Gamma = 0$ ). In Figure 8b, the Courant number is 1.0 requiring only 100 time steps to complete the propagation cycle. In each case, the wave moves too slow as predicted by the phase portrait for higher wave numbers. Additional tests with  $P_{\Delta} = 2$  eliminated the wiggles. When  $P_{\Delta} = 5$ , wiggles were barely perceptible near the peak as shown in Figure 9, where the triangles only represent initial conditions since physical diffusion is now included.

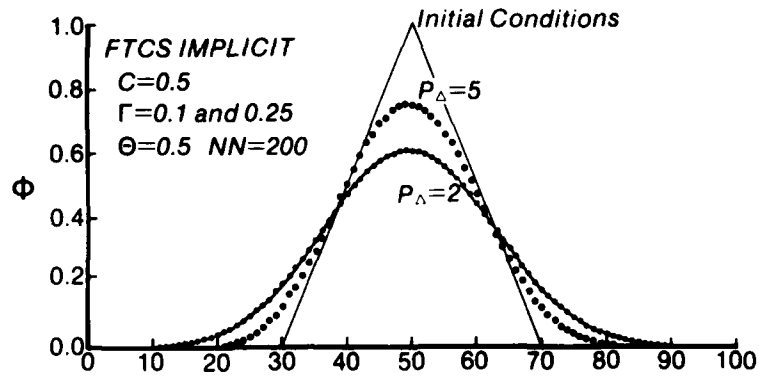


(a) When  $C=0.5$  and after 200 time steps.

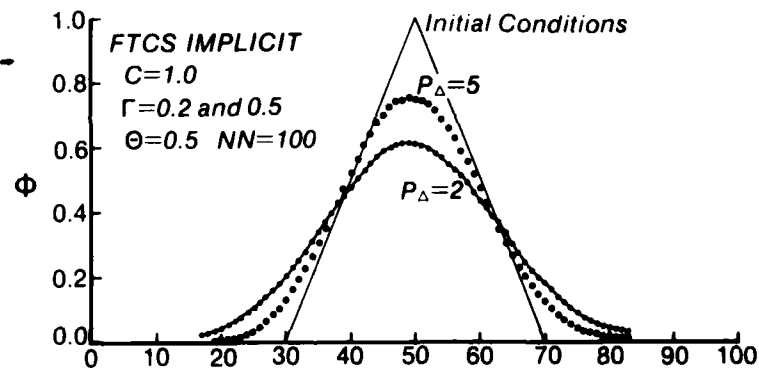


(b) When  $C=1.0$  and after 100 time steps.

Figure 8. Example of wiggle instability for implicit, centered advection of test triangle with periodic boundary conditions



(a) When  $C=0.5$  and after 200 time steps.



(b) When  $C=1.0$  and after 100 time steps.

Figure 9. Suppression of wiggle instability when  $P_{\Delta} \leq 2$  for implicit, centered advection of test triangle. When  $P_{\Delta} = 5$ , a slight oscillation is barely visible

### PART III: IMPLICIT ALGORITHMS

27. Many alternative ways exist to formulate implicit, higher order accurate difference schemes for Equation 1. Two methods are described below, both of which utilize elements of the explicit, Leonard (1979) algorithm.

#### Implicit Leonard Algorithm for Transport-Diffusion (QUICKIST)

28. In discussions of computational efficiency and expense of the QUICK (steady-state) method, Leonard (1979, p. 73) states

Implicit, tridiagonal procedures are similarly economical. In that case, one merely uses (29),\* treating the linear-interpolation term implicitly, with the curvature evaluated as an explicit source term.

As derived in the previous chapter, the linear-interpolation term stems from central differencing the advection term. Consequently, this term is made implicit through use of a weighting coefficient  $\theta$  such that  $0 \leq \theta \leq 1$ , i.e.,

$$(1 - \theta)(\phi_x)_i^n = (1 - \theta) \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} - (1 - \theta) \left[ \phi_{xxx} \frac{\Delta x^2}{3!} + \phi_{xxxx} \frac{\Delta x^4}{5!} + \text{H.O.T.} \right]_i^n \quad (21)$$

$$\theta(\phi_x)_i^{n+1} = \theta \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} - \theta \left[ \phi_{xxx} \frac{\Delta x^2}{3!} + \phi_{xxxx} \frac{\Delta x^4}{5!} + \text{H.O.T.} \right]_i^{n+1} \quad (22)$$

A similar weighting makes the diffusion implicit (Crank-Nicholson method) so that, by analogy to Equation 5,

---

\* Equations 2 and 3 in this report.



$$\begin{aligned}
& \textcircled{1} \left[ \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} \right] + u(1 - \theta) \textcircled{3} \left[ \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} \right] + u\theta \textcircled{7} \left[ \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} \right] \\
& = K(1 - \theta) \textcircled{5} \left[ \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \right] + K\theta \textcircled{9} \left[ \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \right] \\
& \textcircled{2} + \left[ \frac{\Delta t}{2!} \phi_{tt} + \frac{\Delta t^2}{3!} \phi_{ttt} + \frac{\Delta t^3}{4!} \phi_{tttt} + \text{H.O.T.} \right]_i^n \\
& + u(1 - \theta) \textcircled{4} \left[ \frac{\Delta x^2}{3!} \phi_{xxx} + \frac{\Delta x^4}{5!} \phi_{xxxxx} + \text{H.O.T.} \right]_i^n \\
& + u\theta \textcircled{8} \left[ \frac{\Delta x^2}{3!} \phi_{xxx} + \frac{\Delta x^4}{5!} \phi_{xxxxx} + \text{H.O.T.} \right]_i^{n+1} \\
& - K(1 - \theta) \textcircled{6} \left[ \frac{2\Delta x^2}{4!} \phi_{xxxx} + \text{H.O.T.} \right]_i^n - K\theta \textcircled{10} \left[ \frac{2\Delta x^2}{4!} \phi_{xxxx} \right]_i^{n+1} \quad (23)
\end{aligned}$$

When  $\theta = 0$ , terms  $\textcircled{7}$ ,  $\textcircled{8}$ ,  $\textcircled{9}$ , and  $\textcircled{10}$  disappear and the explicit scheme given by Equation 5 is recovered. Again, neglecting all fourth and higher order derivatives, Equation 23 gives, after rearrangement,

(8)

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\theta \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} - u\theta \frac{\Delta x^2}{3!} [\phi_{xxx}]_i^{n+1} - K\theta \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2}$$

$$= -u(1 - \theta) \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + K(1 - \theta) \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}$$

(4)

$$+ u(1 - \theta) \frac{\Delta x^2}{3!} [\phi_{xxx}]_i^n$$

(2a)

(2b)

$$+ \left[ \frac{\Delta t}{2} (u^2 \phi_{xx} - 2uK\phi_{xxx}) \right]_i^n + \left[ \frac{\Delta t^2}{3!} (-u^3 \phi_{xxx}) \right]_i^n \quad (24)$$

29. The numbered brackets identify truncation error terms. Truncation error time derivatives are again converted to space derivatives using Equations 6 and 7 to give terms (2a) and (2b), respectively. All truncation error derivatives are at time level  $n$  except term (8). A third spatial derivative requires four grid points, which is incompatible with a tridiagonal algorithm. Based on the derivation in the previous chapter and the quote above (Leonard 1979, p. 73), for evaluation of the curvature as an "explicit source term," term (8) is taken at time level  $n$ . This is a key assumption in this first method. Also, the time derivative is still centered at grid point  $(i,n)$  so that this implicit method reduces to the explicit method of Leonard (1979) called QUICKEST when  $\theta = 0$ . Here the underlined E also could stand for the explicit algorithm. By analogy, for later reference, this implicit algorithm is labeled QUICKIST.

30. Removing term (8) in Equation 24 to time level  $n$ , multiplying through by  $\Delta t$ , and rearranging by grouping all like terms gives

$$\begin{aligned}
& \left( \frac{C\theta}{2} - \Gamma\theta \right) \phi_{i+1}^{n+1} + (1 + 2\Gamma\theta) \phi_i^{n+1} - \left( \frac{C\theta}{2} + \Gamma\theta \right) \phi_{i-1}^{n+1} \\
& - \left[ -\frac{C(1-\theta)}{2} + \Gamma(1-\theta) \right] \phi_{i+1}^n + \left[ 1 - 2\Gamma(1-\theta) \right] \phi_i^n \\
& + \left[ \frac{C(1-\theta)}{2} + \Gamma(1-\theta) \right] \phi_{i-1}^n + \left[ \frac{C^2 \Delta x^2}{2} \right] [\phi_{xx}]_i^n \\
& + \left[ \frac{C \Delta x^3}{6} (1-\theta) + \underbrace{\frac{C \Delta x^3}{6} \theta}_{(8)} - C \Delta x^3 \Gamma - \frac{C^3 \Delta x^3}{6} \right] [\phi_{xxx}]_i^n \quad (25)
\end{aligned}$$

Note that taking term (8) to level  $n$  effectively removes the influence of  $\theta$  on the truncation errors associated with the convection term.

31. Finally, if again the assumption is made that, inherent in Equation 12 for upstream differencing of left to right flow,  $(\phi_{xxx})_i^n \approx (\phi_{xxx})_{i-1/2}^n$ , then using Equation 11 plus additional rearrangement gives

$$A\phi_{i+1}^{n+1} + B\phi_i^{n+1} + C1\phi_{i-1}^{n+1} = D\phi_{i+1}^n + E\phi_i^n + F\phi_{i-1}^n + H\phi_{i-2}^n \quad (26)$$

Where

$$A = \left( \frac{C\theta}{2} - \Gamma\theta \right) \quad (a)$$

$$B = 1 + 2\Gamma\theta \quad (b)$$

$$C1 = - \left( \frac{C\theta}{2} + \Gamma\theta \right) \quad (c)$$

$$D = \left[ -\frac{C}{2} (1-\theta) + \Gamma(1-\theta) + \frac{C^2}{2} + \frac{C}{6} (1 - C^2 - 6\Gamma) \right] \quad (d)$$

$$E = \left[ 1 - 2\Gamma(1-\theta) - C^2 - \frac{C}{2} (1 - C^2 - 6\Gamma) \right] \quad (e)$$

$$F = \left[ \frac{C}{2} (1-\theta) + \Gamma(1-\theta) + \frac{C^2}{2} + \frac{C}{6} (1 - C^2 - 6\Gamma) \right] \quad (f)$$

$$H = -\frac{C}{6} (1 - C^2 - 6\Gamma) \quad (g)$$

When  $\theta = 0$ , Equation 26 reduces to Equation 15, as expected. This form is convenient for the linear stability analysis and propagation tests using double-sweep, tridiagonal matrix solution procedures.

#### Linear stability analysis of QUICKIST

32. Use of the von Neumann method resulted in the following expression for the amplification factor

$$A(\alpha) = \frac{D \exp(\overset{\circ}{\Pi}\alpha) + E + F \exp(-\overset{\circ}{\Pi}\alpha) + H \exp(-\overset{\circ}{\Pi}2\alpha)}{A \exp(\overset{\circ}{\Pi}\alpha) + B + C1 \exp(-\overset{\circ}{\Pi}\alpha)} \quad (27)$$

A simple computer program written in complex arithmetic was employed to find  $|A|$  and  $Q$  over 30 values of  $\alpha$  from Equation 27 without further simplification.

33. Some results when  $\theta = 0.5$  are shown in Figure 10 for  $C = 0.5$  and Figure 11 when  $C = 1.0$ . In both instances, the explicit

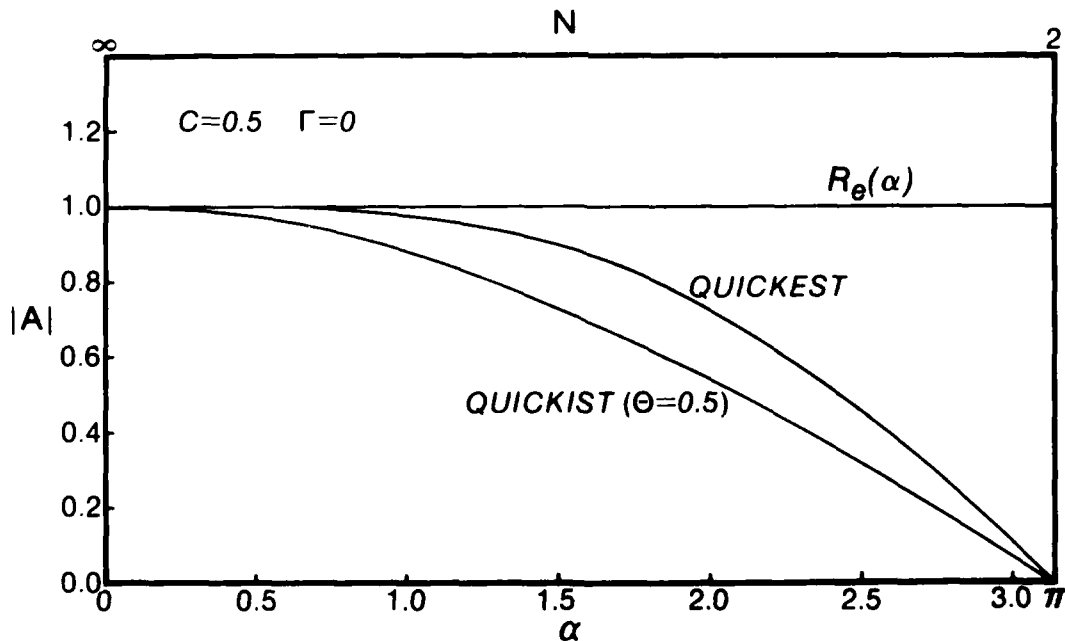


Figure 10. Amplitude portrait for QUICKEST versus QUICKIST schemes when  $C = 0.5$ ,  $\Gamma = 0$ . Both have no phase errors for all of  $\alpha$

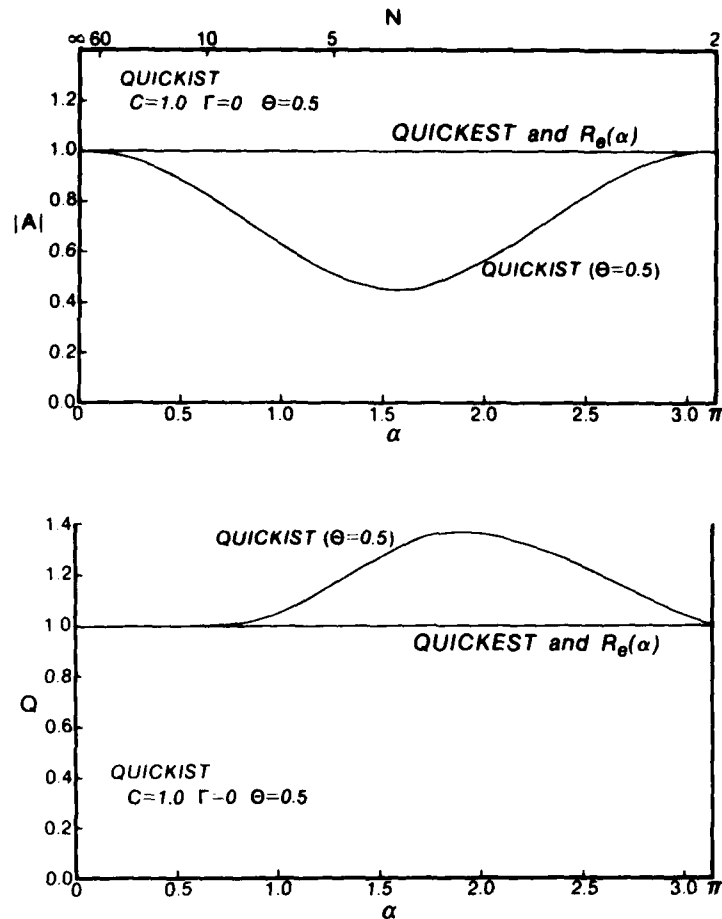


Figure 11. Amplitude and phase portraits for QUICKEST and QUICKIST schemes when  $C = 1.0$ ,  $\Gamma = 0$

scheme is more accurate for pure advection. The extent of numerical damping when  $C = 1.0$  for the QUICKIST algorithm can be considered excessive. However, as shown in Figure 4 for  $C = 0.5$ ,  $\Gamma = 1.1$ , QUICKIST ( $\theta = 0.5$ ) appears more accurate for all  $\alpha$ . Figure 5 also reveals that when  $C$  is again 0.5 but  $\Gamma$  now 1.2, QUICKIST is stable whereas the explicit scheme is unstable. The implicit algorithm has far superior phase response for these latter examples. Finally, Figure 12 reveals that the explicit scheme is more accurate over all  $\alpha$  for the pure diffusion case when  $\Gamma = 1/6$ .

34. The  $(\Gamma, C)$  plane was mapped for the implicit scheme to

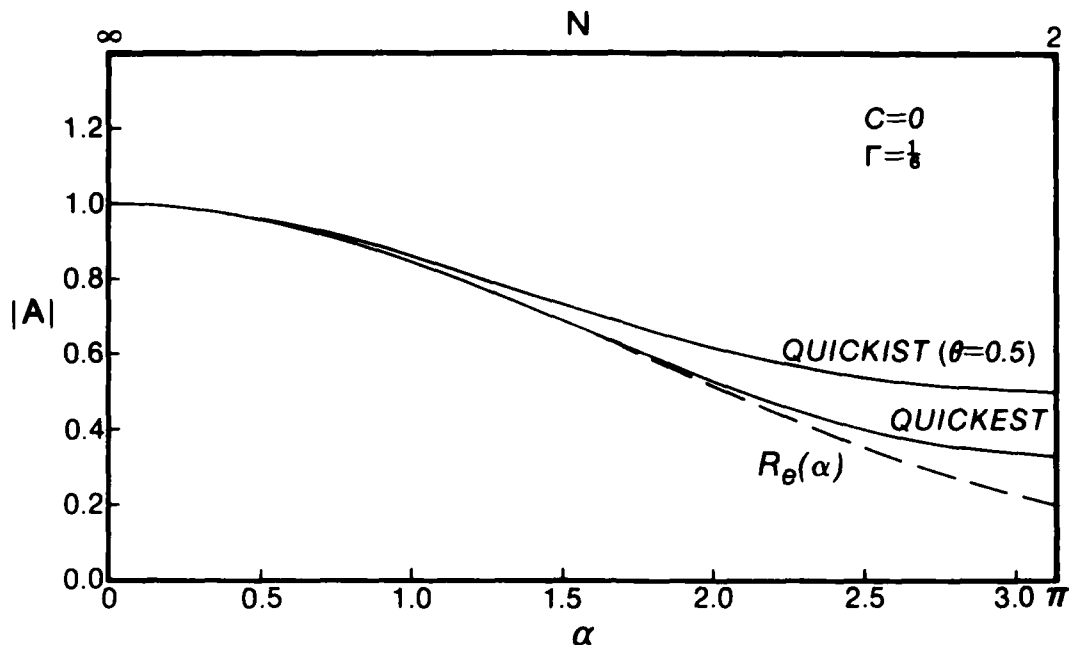


Figure 12. Amplitude response for pure diffusion ( $C = 0$ ) when  $\Gamma = 1/6$  for both QUICKEST and QUICKIST schemes

determine its stability range\* for comparison with Leonard's results in Figure 3. The results were somewhat disappointing. It was anticipated that the implicit QUICKIST algorithm would have a much larger stable region than shown in Figure 13. However, the unstable corner below  $C = 0.5$  and beyond  $\Gamma = 0.5$  was eliminated. The stable range of QUICKEST method is also shown in Figure 13 for comparison.

35. The amplitude accuracy of QUICKIST was characterized in the stable range out to  $\Gamma = 1.3$  using the RMS difference norm, as before. Figure 14 presents the "contour" map of RMS difference values and gives a weighted-average value in the stable area (arbitrarily,  $\Gamma \leq 1.3$ ) of 0.0946. As expected, QUICKIST with  $\theta = 0.5$  is less accurate than the explicit Leonard algorithm.

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\*  $|A| > 1.001$  for any  $0 \leq \alpha \leq \pi$  was the criteria employed.

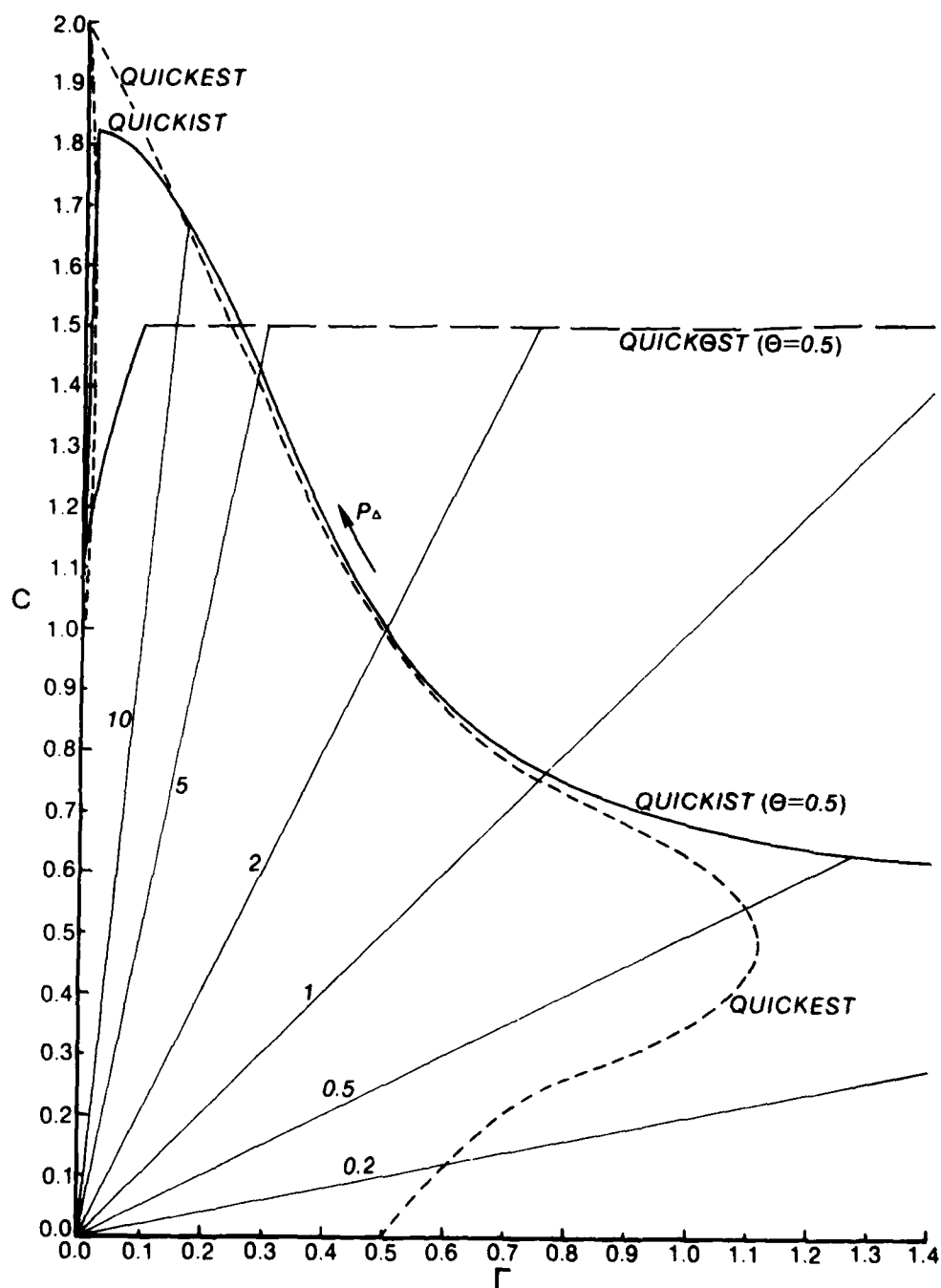


Figure 13. Stable range of QUICKIST method in  $(\Gamma, C)$  plane as determined in this study. Also shown is stable range of QUICKEST scheme and the QUICKΘST algorithm described later in this report

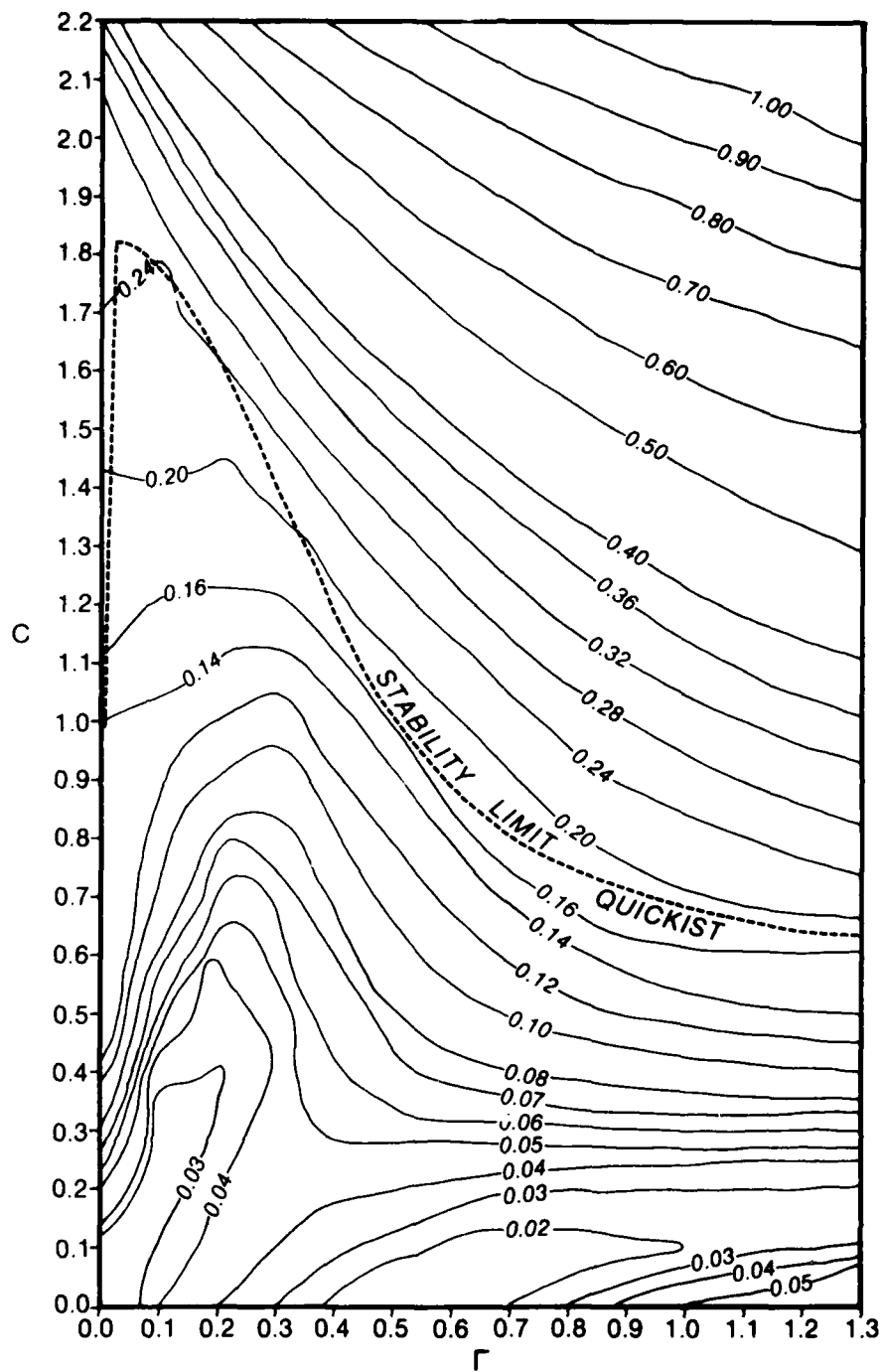
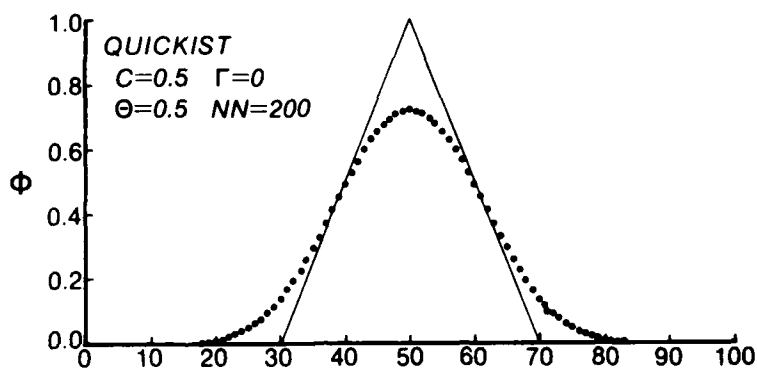


Figure 14. Iso-amplitude lines of equal RMS difference values in  $(\Gamma, C)$  plane for QUICKIST. Stability range also shown

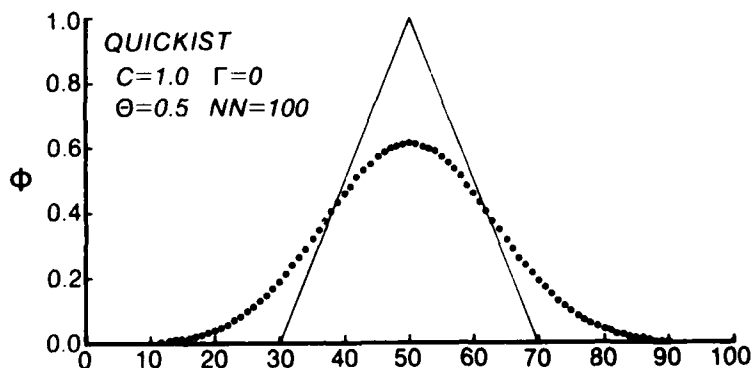


### Propagation tests of QUICKIST

36. The QUICKIST inaccuracies are confirmed by results of the triangle propagation tests. Excessive numerical damping results to the extent demonstrated in Figure 15 for  $C = 0.5$  (Fig. 15a) and  $C = 1.0$  (Fig. 15b). When compared with Figure 7 and the fact that  $C = 1.0$  gives an exact result for the explicit scheme, it must be concluded that the implicit QUICKIST algorithm is too inaccurate to warrant further study.



(a) When  $C=0.5$  and after 200 time steps.



(b) When  $C=1.0$  and after 100 time steps.

Figure 15. Propagation tests for pure advection using periodic boundary conditions and QUICKIST algorithm.  
Large numerical diffusion present

### Fully Centered, Implicit Algorithm (QUICK0ST)

37. The inaccuracy of the QUICKIST algorithm can be traced to the off-centering of the  $\phi_t$  derivative at (i,n). The sole advantage of this method is that when  $\theta = 0$ , the explicit QUICKEST algorithm is regained.

38. A fully centered, implicit method would utilize grid point (i,n + 1/2) in the Taylor series expansion so that even the  $\phi_t$  derivative is effectively weighted by  $\theta$ . When  $\theta = 0$ , the explicit QUICKEST scheme would no longer be recovered. However, far greater numerical accuracy is anticipated since all terms and truncation errors are centered at the same time level by  $\theta$ . Consequently, this fully centered implicit Leonard scheme is given the acronym QUICK0ST.

#### Derivation

39. Consider the schematic grid sketched in Figure 16. A two-dimensional Taylor expansion of the form

$$\begin{aligned} f(a + h, b + k) = f(a,b) + \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial t} \right) f(x,t) \Big|_{\substack{x=a \\ t=b}} \\ + \frac{1}{n!} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial t} \right)^n f(x,t) \Big|_{\substack{x=a \\ t=b}} + \dots \end{aligned} \quad (28)$$

is utilized where

$$\begin{aligned} a &= i \\ b &= n + 1/2 \\ h &= \Delta x \\ k &= \Delta t/2 \end{aligned} \quad (29)$$

for the nomenclature in Figure 16. The initial expansion<sup>\*</sup> about (i,n + 1/2) yields by analogy with Equation 23

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\* A coefficient was discovered to be missing in this expansion at a later date. The complete results for the correct expansion are given in Appendix A. Surprisingly, the correct expansion (QUICK0ST 2 exhibited little if any improvement over the original explicit scheme QUICKEST. Therefore, it was dropped in favor of the "chance" algorithm QUICK0ST discussed in detail herein. It was not possible to determine the cause for this unexpected result within the allotted scope of the study.

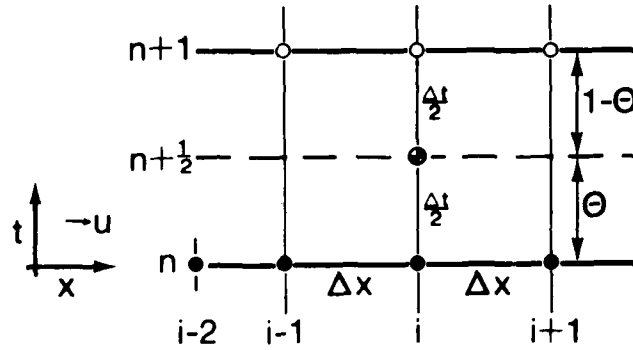


Figure 16. Schematic of operator for QUICKθST scheme determination

$$\begin{aligned}
 & \textcircled{1} \left[ \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} \right] + u(1 - \theta) \textcircled{3} \left[ \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} \right] + u\theta \textcircled{7} \left[ \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} \right] \\
 & = K(1 - \theta) \textcircled{5} \left[ \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \right] + K\theta \textcircled{9} \left[ \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \right] \\
 & + \textcircled{2} \left[ -\frac{1}{24} \Delta t^2 \phi_{ttt} + \text{H.O.T.} \right]_i^{n+1/2} \\
 & + u(1 - \theta) \textcircled{4} \left[ -\frac{1}{2!} \frac{\Delta t}{2} \phi_{xt} + \frac{1}{3!} \Delta x^2 \phi_{xxx} + \frac{\Delta t^2}{24} \phi_{xtt} + \text{H.O.T.} \right]_i^{n+1/2} \\
 & + u\theta \textcircled{8} \left[ \frac{1}{2!} \frac{\Delta t}{2} \phi_{xt} + \frac{1}{3!} \Delta x^2 \phi_{xxx} + \frac{\Delta t^2}{24} \phi_{xtt} + \text{H.O.T.} \right]_i^{n+1/2}
 \end{aligned}$$

(6)

$$- K(1 - \theta) \left[ \frac{1}{3!} \Delta t \phi_{xxt} + \text{H.O.T.} \right]_i^{n+1/2}$$

(10)

$$- K\theta \left[ \frac{1}{3!} \Delta t \phi_{xxt} + \text{H.O.T.} \right]_i^{n+1/2} \quad (30)$$

The truncation error terms (2), (4), (6), (8), and (10) are now centered at  $(i, n + 1/2)$  giving different coefficients and incorporating mixed time/space derivatives. Neglecting all fourth and higher order derivatives; using Equations 6, 7, and 8 to convert all time and mixed-time derivatives to pure space derivatives; and combining all like derivatives for truncation errors yields

$$\begin{aligned} & \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u(1 - \theta) \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + u\theta \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} \\ &= K(1 - \theta) \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + K\theta \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \\ & \quad + \left[ \frac{u^2 \Delta t}{4} (1 - 2\theta) \right] (\phi_{xx})_i^{n+1/2} \\ & \quad + \left[ \frac{u \Delta x^2}{6} - \frac{5Ku(1 - 2\theta)\Delta t}{12} \right] (\phi_{xxx})_i^{n+1/2} \end{aligned} \quad (31)$$

In Equation 31, truncation error from terms (4) and (8) contribute to  $\phi_{xx}$  while all truncation error terms contribute to the  $\phi_{xxx}$  coefficient.

40. It is now assumed that:

- a. The truncation errors in Equation 31 are evaluated at time level  $n$ .
- b. The  $\phi_{xxx}$  term is centered upstream (grid point  $(i - 1/2)$  for left to right flow).

Assumption a is required for  $\phi_{xxx}$  to retain the tridiagonal structure of the algorithm as in QUICKIST. Also, it is felt that for consistency,  $\phi_{xx}$  should also be taken at level  $n$ . Assumption b follows from Part II to produce the quadratic, higher order, accurate, upstream difference operator for advection. Using these two assumptions and making the usual rearrangements gives

$$A\phi_{i+1}^{n+1} + B\phi_i^{n+1} + C\phi_{i-1}^{n+1} = D\phi_{i+1}^n + E\phi_i^n + F\phi_{i-1}^n + H\phi_{i-2}^n \quad (32)$$

where

$$A = \frac{C\theta}{2} - \Gamma\theta \quad (a)$$

$$B = 1 + 2\Gamma\theta \quad (b)$$

$$C = -\left(\frac{C\theta}{2} + \Gamma\theta\right) \quad (c)$$

$$D = \left[ -\frac{C}{2}(1 - \theta) + \Gamma(1 - \theta) + \frac{C^2}{4}(1 - 2\theta) + \frac{C}{6} - \frac{5}{12}C\Gamma(1 - 2\theta) \right] \quad (d)$$

$$E = \left[ 1 - 2\Gamma(1 - \theta) - \frac{C^2}{2}(1 - 2\theta) - \frac{C}{2} + \frac{15}{12}C\Gamma(1 - 2\theta) \right] \quad (e)$$

$$F = \left[ \frac{C}{2}(1 - \theta) + \Gamma(1 - \theta) + \frac{C^2}{4}(1 - 2\theta) + \frac{C}{2} - \frac{15}{12}C\Gamma(1 - 2\theta) \right] \quad (f)$$

$$H = -\left[ \frac{C}{6} - \frac{5}{12}C\Gamma(1 - 2\theta) \right] \quad (g)$$

The coefficients  $D$ ,  $E$ ,  $F$ , and  $H$  in Equation 32 are different from the first implicit scheme given by Equation 26. As an example, consider the coefficients when  $C = 1.0$ ,  $\Gamma = 0$ ,  $\theta = 0.5$

QUICKØST

$$\frac{1}{4}\phi_{i+1}^{n+1} + \phi_i^{n+1} - \frac{1}{4}\phi_{i-1}^{n+1} = -\frac{1}{12}\phi_{i+1}^n + \frac{6}{12}\phi_i^n + \frac{9}{12}\phi_{i-1}^n - \frac{2}{12}\phi_{i-2}^n \quad (a)$$

#### QUICKIST

$$\frac{1}{4} \phi_{i+1}^{n+1} + \phi_i^{n+1} - \frac{1}{4} \phi_{i-1}^{n+1} = \frac{1}{4} \phi_{i+1}^n + \frac{3}{4} \phi_{i-1}^n \quad (b) \quad (33)$$

#### QUICKEST ( $\theta = 0$ )

$$\phi_i^{n+1} = \phi_{i-1}^n \quad (c)$$

It appears that QUICK0ST retains more of the intended upstream interpolation flavor of the Leonard QUICK method.

#### Linear stability analysis of QUICK0ST

41. Equation 27 is again employed but with coefficients calculated from Equation 32. Some results ( $\theta = 0.5$ ) are shown in Figure 17. This implicit scheme is exact in amplitude response for all  $\alpha$  when  $C = 1.0$  or  $0.5$  for pure advection. Some phase errors exist for higher wave numbers as demonstrated in Figure 17(b). Figure 17 when compared with Figures 10 and 11 reveals that QUICK0ST is vastly superior to QUICKIST and similar to the explicit scheme for these Courant numbers. Both implicit schemes reduce to the Crank-Nicholson scheme for pure diffusion ( $C = 0$ ,  $\theta = 0.5$ ).

42. Mapping the stable area of QUICK0ST in the  $(\Gamma, C)$  plane revealed a much larger and uniformly stable region as shown previously in Figure 13. QUICK0ST is stable for all  $\Gamma$  below  $C = 1.5$  except in the small area above  $C = 1.0$  near the ordinate.

43. The amplitude accuracy of QUICK0ST is summarized in Figure 18 out to  $\Gamma = 1.3$  again using the RMS difference as norm. The weighted-average value in the enlarged stable area ( $\Gamma \leq 1.3$ ) is

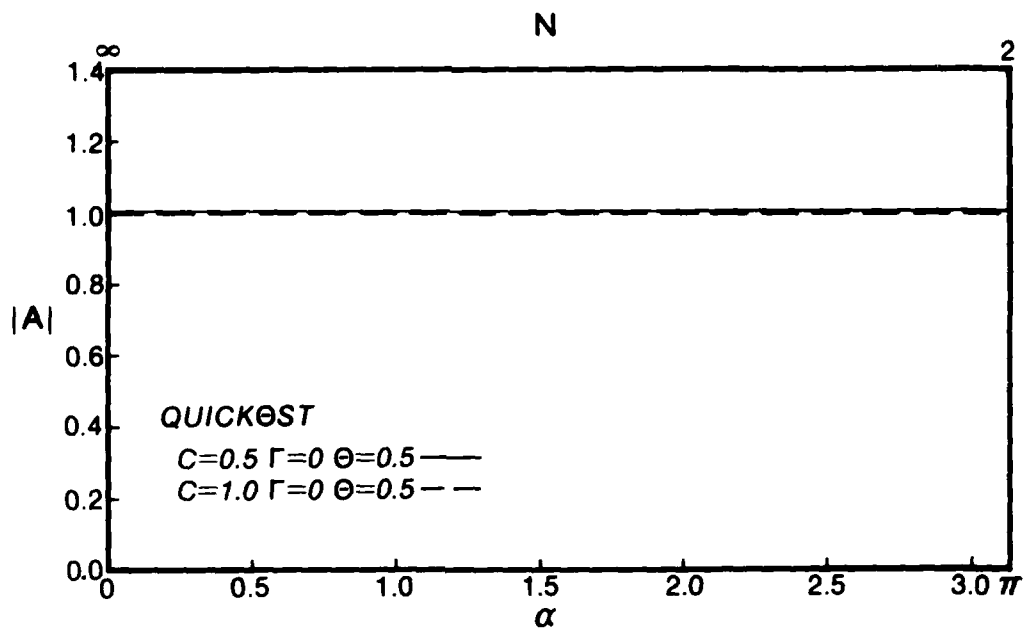
<u>QUICK0ST</u>	0.0890
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and, for comparison,

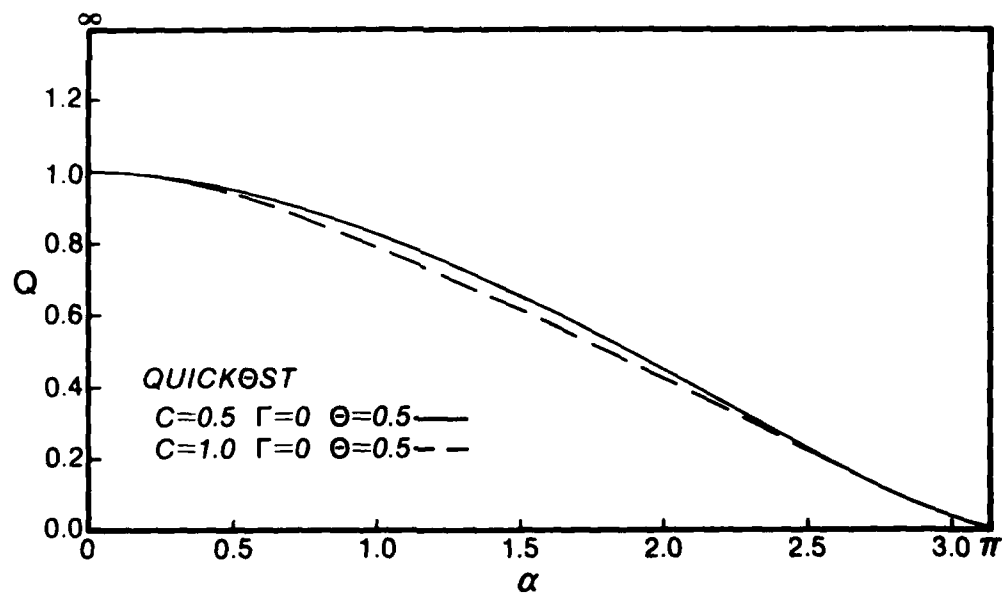
<u>QUICKIST</u>	0.0946
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<u>QUICKEST</u>	0.0568
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As expected, the QUICK0ST algorithm is more accurate in amplitude response over all wave numbers than QUICKIST. It is generally more inaccurate than the explicit scheme, but is far more useful due to



(a) Scheme is exact in amplitude response.



(b) Some phase errors present.

Figure 17. Amplitude and phase portraits for QUICK $\Theta$ ST scheme and pure advection ( $\Gamma = 0$ ) case when  $C = 0.5$  and  $1.0$

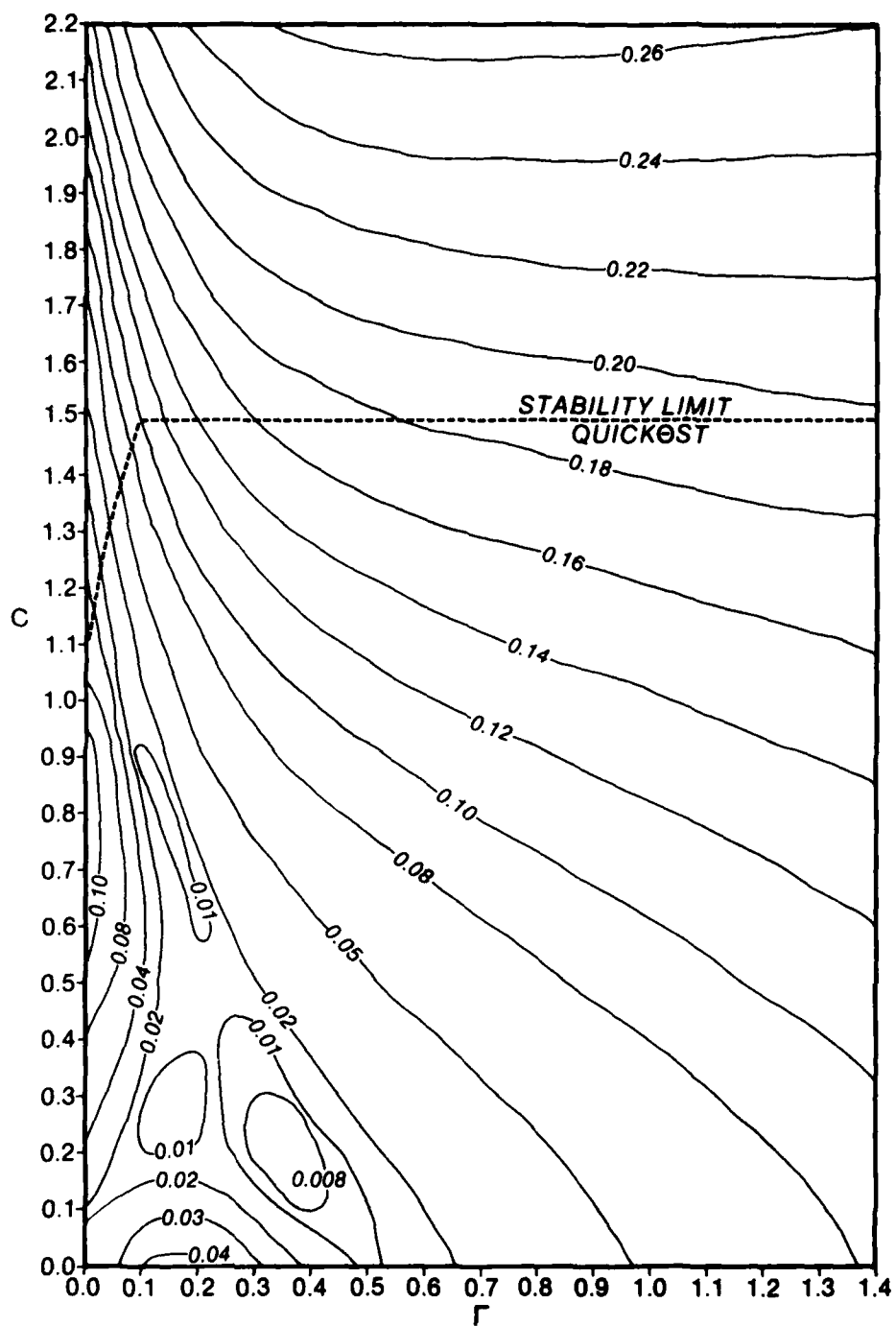


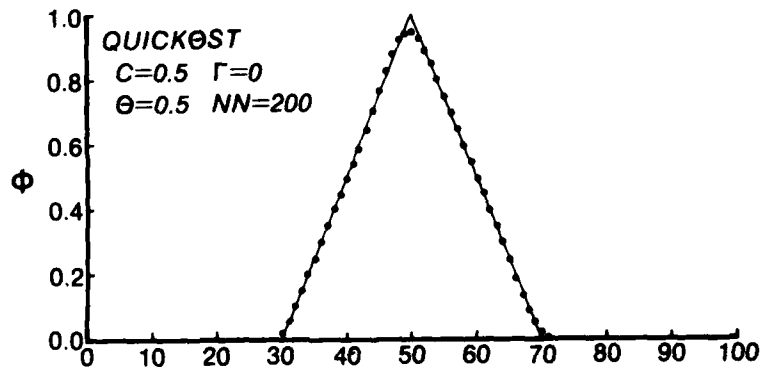
Figure 18. Iso-amplitude plot for QUICKØST with stable range also shown



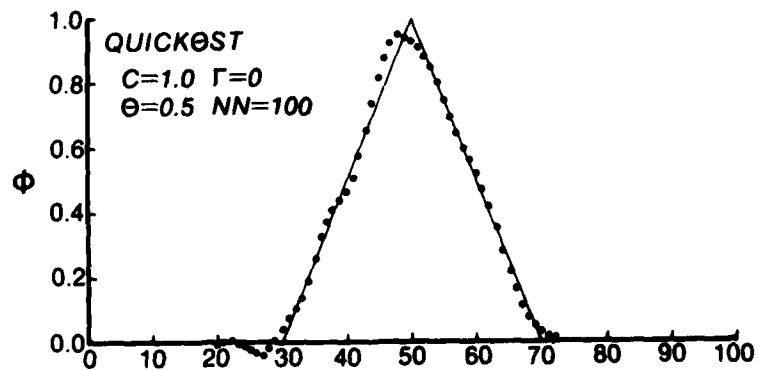
the extended stable region above  $C = 1.0$  for practical values of  $\Gamma > 0.5$ . The phase accuracy for the three schemes generally followed these same trends.

#### Propagation tests of QUICK $\theta$ ST

44. The excellent numerical accuracy of the QUICK $\theta$ ST is confirmed by the triangle propagation test results depicted in Figure 19. The discrepancy at the peak is comparable to that produced by the explicit scheme (Figure 7) and the waviness of the upstream face is due to phase errors (recall Figure 17). The closeness of numerical results between the explicit and QUICK $\theta$ ST algorithms is also demonstrated in Figures 20 and 21 where some physical diffusion ( $\Gamma = 0.1$ ) is now present.

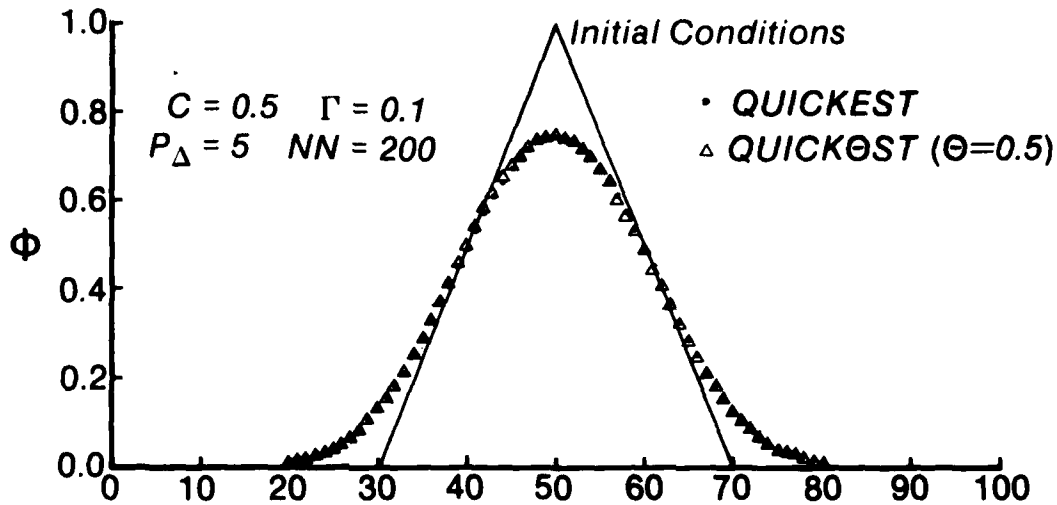


(a) When  $C=0.5$  and after 200 time steps.

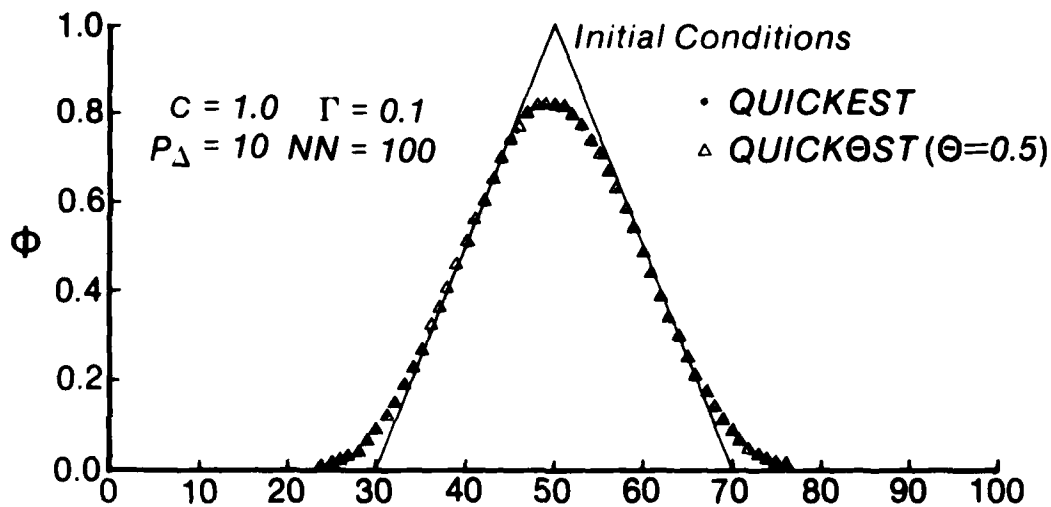


(b) When  $C=1.0$  and after 100 time steps.

Figure 19. Propagation test results for pure advection case using periodic boundary conditions and QUICK $\theta$ ST algorithm



(a) When  $C=0.5$ ,  $\Gamma=0.1$ ,  $P_{\Delta}=5$  and after 200 time steps.



(b) When  $C=1.0$ ,  $\Gamma=0.1$ ,  $P_{\Delta}=10$  and after 100 time steps.

Figure 20. Propagation test results for example with some physical diffusion present ( $\Gamma = 0.1$ ) comparing explicit (dots) and implicit (triangles) QUICKΘST algorithms

In these examples, only initial conditions are shown.

45. Other propagation tests gave similar results.

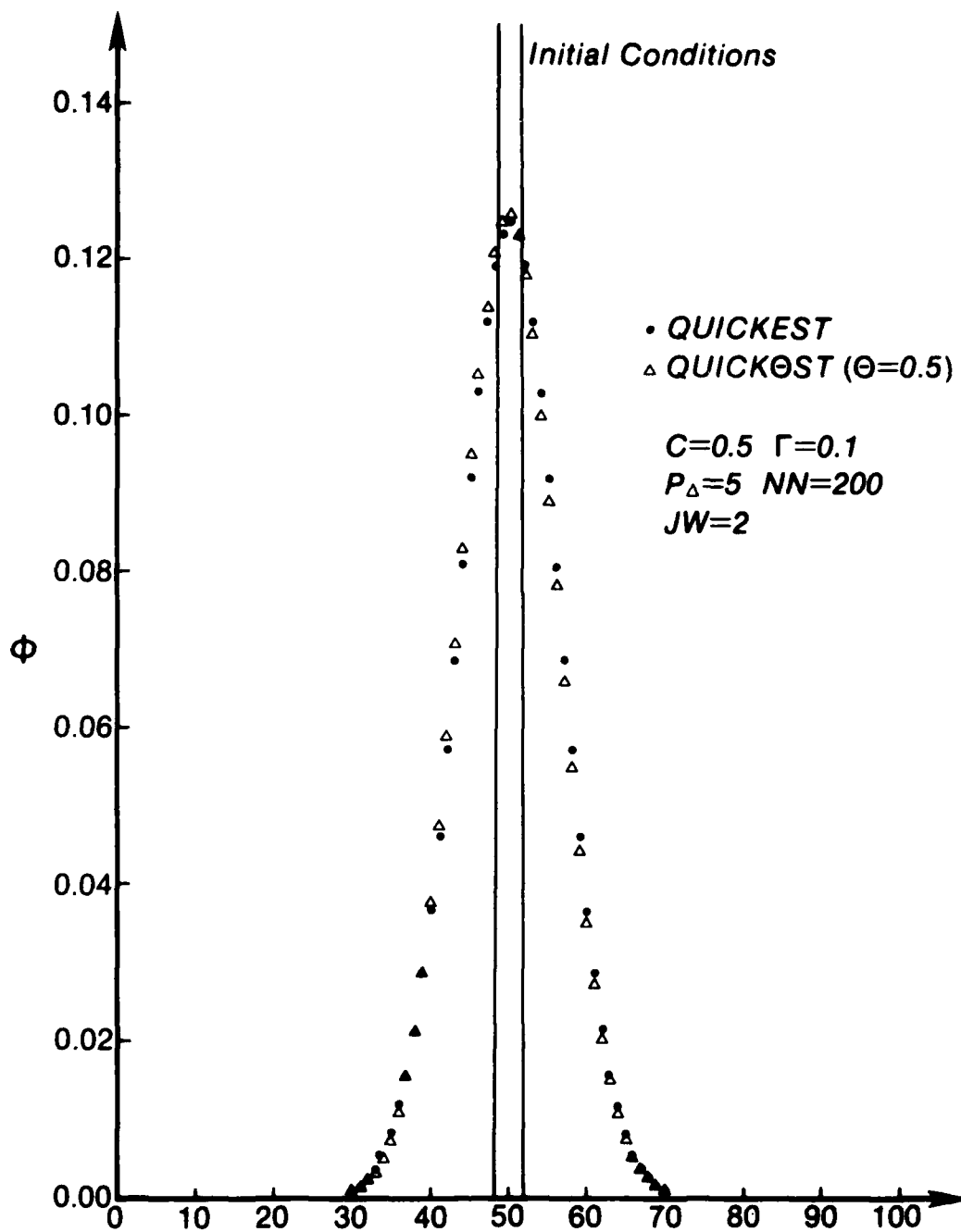


Figure 21. Propagation test results for narrow triangle ( $JW = 2$ ) and physical diffusion ( $\Gamma = 0.1$ ) comparing QUICKEST (dots) and QUICKΘST (triangles) algorithm when  $C = 0.5$ ,  $\Gamma = 0.1$ ,  $P_{\Delta} = 5$  after 200 time steps

## PART IV: CONCLUSIONS AND RECOMMENDATIONS

46. The purpose of this project was to develop and study numerical properties of an implicit algorithm consistent with the QUICKEST scheme of Leonard (1979) for the unsteady, one-dimensional transport-diffusion equation. Based upon the results discussed in this report, the following conclusions are drawn and recommendations offered.

### Conclusions

47. The explicit algorithm labeled QUICKEST is identical to a forward-time, centered-space scheme with all truncation errors expressed as spatial derivatives and removed through  $\phi_{xx}$  and  $\phi_{xxx}$  terms. The  $\phi_{xxx}$  term is centered upstream and results in a higher order, accurate, upstream difference method.

48. A fully centered, implicit scheme called QUICK $\theta$ ST, as developed herein, is of comparable accuracy to the explicit operator yet extends the stable range in the  $(\Gamma, C)$  plane to essentially below the line,  $C = 1.5$  for all  $\Gamma$ .

49. QUICK $\theta$ ST is a stable, accurate, and robust algorithm of considerable engineering usefulness for transport-diffusion computations.

50. Because development of the implicit QUICK $\theta$ ST algorithm has proven to be highly successful, further research on the QUICK $\theta$ ST 2 scheme is not warranted except to learn the reasons for its poor performance.

### Recommendations

51. The QUICK $\theta$ ST scheme for one-dimensional flows should be extended to variable grid spacing. Only nomenclature and programming modifications are required.

52. A two-dimensional QUICK $\theta$ ST algorithm should be developed. Use of an alternating-direction implicit (ADI) structure should be considered along with the "double-sweep" solution algorithm.

53. An experimental test program must be devised to fully verify the two-dimensional QUICK0ST against existing and new data from both the field and the laboratory.

54. Systems-oriented computer codes and extensive software should be written for ease in application by computational hydraulic engineers.

## REFERENCES

- Abbott, M. B. 1979. Computational Hydraulics, Pitman, London.
- Leonard, B. P. 1979. "A Stable and Accurate Convective Modelling Procedure Based on Quadratic Upstream Interpolation," Computer Methods in Applied Mechanics and Engineering, Vol 19, pp 59-98.
- Reid, R. O., and Basco, D.R. 1982. "Numerical Convolution for Solution of Wave Propagation Problems: Filter Scheme Methods," Journal of Hydraulic Research (to be published).
- Roache, P. J. 1977. Computational Fluid Dynamics, Hermosa, Albuquerque, N. Mex.

## APPENDIX A: DERIVATION OF QUICK0ST 2

1. As mentioned in the footnote on page 37, the original expansion to develop the QUICK0ST algorithm discussed in this report was found to be incorrect (Ross Hall, 19 Oct. 1982, personal communication). This Appendix gives the explanation, all corrected equations, and a linear stability analysis of the results. This corrected version is dubbed QUICK0ST 2 and is shown to be a far less robust algorithm than the "chance" algorithm QUICK0ST. For this reason, the original report and all conclusions were felt to still be valid and the corrected algorithm QUICK0ST 2 relegated to this Appendix.

2. Consider the schematic operator shown in Figure 16. The general two-dimensional Taylor series expansion given in Equation 28 is correct but the indices should be

$$\begin{aligned} a &= i \\ b &= n+\theta \\ h &= \pm \Delta x \\ k &= +(1-\theta)\Delta t, -\theta\Delta t \end{aligned} \tag{A1}$$

This will give, for example, a space difference from  $n+\theta$  to  $n+1$  (over  $+(1-\theta)\Delta t$ ) and from  $i$  to  $i+1$  (over  $+\Delta x$ )

$$\begin{aligned} \phi_{i+1}^{n+1} &= \phi_i^{n+\theta} + [\Delta x (\phi_x)_i^{n+\theta} + (1-\theta)\Delta t (\phi_t)_i^{n+\theta}] \\ &+ \frac{1}{2!} [\Delta x^2 (\phi_{xx})_i^{n+\theta} + (1-\theta)^2 \Delta t^2 (\phi_{tt})_i^{n+\theta} + 2\Delta x (1-\theta)\Delta t (\phi_{xt})_i^{n+\theta}] \\ &+ \frac{1}{3!} [\Delta x^3 (\phi_{xxx})_i^{n+\theta} + 3\Delta x^2 (1-\theta)\Delta t (\phi_{xxt})_i^{n+\theta} \\ &+ 3\Delta x (1-\theta)^2 \Delta t^2 (\phi_{xtt})_i^{n+\theta} + (1-\theta)^3 \Delta t^3 (\phi_{ttt})_i^{n+\theta}] \end{aligned} \tag{A2}$$

The coefficients underlined in Equation A2, namely the 2 and 3, were inadvertently left out of this and all other expansions in the original derivation that produced the "chance" algorithm QUICKST.

3. The correct expansion gives the following equations.

Corrected Equation 30 (pp 38-39)

$$\begin{aligned}
 & \begin{matrix} (1) & (3) & (7) \\ \left[ \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} \right] + u(1-\theta) \left[ \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} \right] + u\theta \left[ \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} \right] \\ \\ (5) & (9) \\ = K(1-\theta) \left[ \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \right] + K\theta \left[ \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \right] \\ \\ (2) \\ + \left[ \frac{(1-2\theta)\Delta t}{2!} (\phi_{tt}) + \frac{(1-3\theta+3\theta^2)\Delta t^2}{3!} (\phi_{ttt}) + \text{H.O.T.} \right]_i^{n+\theta} \\ \\ (4) \\ -u(1-\theta) \left[ \theta\Delta t (\phi_{xt}) - \frac{1}{3!}\Delta x^2 (\phi_{xxx}) - \frac{3}{3!}\theta^2\Delta t^2 (\phi_{xtt}) + \text{H.O.T.} \right]_i^{n+\theta} \\ \\ (8) \\ +u\theta \left[ (1-\theta)\Delta t (\phi_{xt}) + \frac{1}{3!}\Delta x^2 (\phi_{xxx}) + \frac{3}{3!}(1-\theta)^2\Delta t^2 (\phi_{xtt}) + \text{H.O.T.} \right]_i^{n+\theta} \\ \\ (6) & (10) \\ +K(1-\theta) \left[ \frac{6\theta\Delta t}{3!} (\phi_{xxt}) + \text{H.O.T.} \right]_i^{n+\theta} - K\theta \left[ \frac{6(1-\theta)\Delta t}{3!} (\phi_{xxt}) + \text{H.O.T.} \right]_i^{n+\theta} \quad (A3) \end{matrix}
 \end{aligned}$$

Corrected Equation 31 (p 39)

$$\begin{aligned}
 & \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u(1-\theta) \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} + u\theta \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} \\
 & = K(1-\theta) \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + K\theta \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \\
 & \quad (2) \\
 & + \left[ \frac{u^2\Delta t}{2} (1-2\theta) \right] (\phi_{xx})_i^{n+\theta}
 \end{aligned}$$



(2)+(4)+(6)

$$\left[ \frac{u\Delta x^2}{6} - \frac{(1-6\theta+6\theta^2)u^3\Delta t^2}{6} - (1-2\theta)uK\Delta t \right] (\phi_{xxx})_i^{n+\theta} \quad (A4)$$

where Term (8) + Term (10)  $\equiv 0$

Corrected Coefficients in Equation 32 (p 40)

$$A = \frac{C\theta}{2} - r\theta - R\theta$$

$$B = 1 + 2r\theta + 2R\theta$$

$$C1 = -\left(\frac{C\theta}{2} + r\theta + R\theta\right)$$

$$D = -\frac{C(1-\theta)}{2} + r(1-\theta) + R(1-\theta) + S$$

$$E = 1 - 2r(1-\theta) - 2R(1-\theta) - 3S$$

$$F = +\frac{C(1-\theta)}{2} + r(1-\theta) + R(1-\theta) + 3S$$

$$H = -S$$

(A5)

where:

$$R = \frac{C^2}{2} (1-2\theta)$$

$$S = \left[ \frac{C}{6} - \frac{(1-6\theta+6\theta^2)}{6} C^3 - (1-2\theta)Cr \right] \quad (A5)$$

Corrected Equation 33a (p 40) when C=1.0, r=0,  $\theta=0.5$ , QUICK $\theta$ ST 2

$$\frac{1}{4} \phi_{i+1}^{n+1} + \phi_i^{n+1} - \frac{1}{4} \phi_{i-1}^{n+1} = 0 \cdot \phi_{i+1}^n + \frac{1}{4} \phi_i^n + \phi_{i-1}^n - \frac{1}{4} \phi_{i-2}^n \quad (A6)$$

4. A linear stability analysis of QUICK $\theta$ ST 2 using Equation 27 was employed but with coefficients calculated from Equation A5 above. Some results are summarized below for a perfectly centered scheme with  $\theta=0.5$ .

<u>C</u>	<u>r</u>	<u>Remarks</u>
1.0	0	Exact for all $\alpha$
0.75	0	Stable
0.5	0	Stable
1.0	1.0	Stable

<u>C</u>	<u><math>\Gamma</math></u>	<u>Remarks</u>
1.01	1.0	Unstable
1.5	0	Unstable
2.0	0.5	Unstable

5. The scheme QUICK $\theta$ ST 2 becomes unstable for all  $\Gamma$  when the Courant number exceeds unity which is an unexpected result for an implicit scheme. Using other values of  $\theta$  (0.4, 0.51, 0.75, 1.0) produced erratic results with a stable region always far smaller than that given by the QUICK $\theta$ ST scheme. We conclude that this algorithm is far less robust and inferior to the QUICK $\theta$ ST algorithm discussed in this report.

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